Supplementary Materials

A Comprehensive Computational NMR Analysis of Organic Polyarsenicals Including the Marine Sponge-Derived Arsenicins A-D and Their Synthetic Analogs

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Table S1. Calculated ^{1}H-NMR chemical shifts of polyarsenicals **1**-**12** in chloroform by using combinations of methods (GIAO, CSGT), functionals (OLYP, M06-L, PBE1PBE, TPSSh**)** and the indicated basis sets; experimental values in $CDCl_3$ for comparison, in redline. For the numbering of H and C atoms, see structures in Figure S1.

			OLYP									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**H6 e H9**	2.42	2.36	2.16	2.27	2.30	2.13	2.03	2.23	1.91	2.19	2.04
	H2 e H3	2.23	2.17	1.97	2.09	2.10	1.93	1.84	2.02	1.74	1.99	1.86
	H5 e H8	1.37	1.28	1.09	1.18	1.20	1.00	0.91	1.10	0.80	1.04	0.91
2	**H2-H4-H13-H14**	1.85	1.88	1.66	1.75	1.78	1.60	1.48	1.69	1.35	1.64	1.46
3	**H12-H13**	2.71	2.78	2.55	2.64	2.66	2.52	2.38	2.60	2.26	2.57	2.38
	H11-H14	1.71	1.75	1.53	1.61	1.63	1.45	1.33	1.54	1.21	1.49	1.32
4	**H3-H6-H8**	3.11	3.11	2.89	3.03	3.04	2.92	2.81	3.01	2.69	2.99	2.83
	H2-H5-H9	1.53	1.50	1.32	1.41	1.44	1.25	1.16	1.34	1.05	1.27	1.15
5	**H2-H4**	1.40	1.12	0.86	0.98	1.02	0.79	0.83	0.933	0.67	0.93	0.83
	C*H*$_3$	1.59	1.62	1.50	1.56	1.58	1.43	1.46	1.56	1.37	1.52	1.45
6	**H14**	3.96	3.89	3.66	3.90	3.92	3.69	3.54	3.83	3.53	3.71	3.52
	H12	3.46	3.42	3.20	3.43	3.43	3.22	3.10	3.37	3.09	3.24	3.08
	H10	3.44	3.20	2.92	3.17	3.15	2.99	2.78	3.14	2.76	3.01	2.75
	H15	2.34	2.19	1.87	2.03	2.03	1.91	1.74	1.99	1.65	1.86	1.63
	H13	1.92	1.76	1.50	1.63	1.65	1.52	1.39	1.61	1.30	1.50	1.32
	H11	1.56	1.35	1.07	1.20	1.20	1.08	0.93	1.17	0.82	1.05	0.83
7	**H14**	3.50	3.43	3.19	3.41	3.43	3.24	3.43	3.38	3.08	3.27	3.10
	H10	3.27	3.07	2.81	3.04	3.02	2.88	3.01	3.02	2.66	2.91	2.68
	H12	2.99	2.95	2.74	2.95	2.94	2.77	2.97	2.91	2.62	2.79	2.64
	H15	2.02	1.79	1.52	1.64	1.66	1.55	1.70	1.63	1.30	1.48	1.28
	H13	1.44	1.21	0.98	1.09	1.11	0.98	1.18	1.07	0.78	0.95	0.81
	H11	1.29	1.01	0.76	0.87	0.89	0.76	0.93	0.85	0.53	0.71	0.54
8	**H11-H14**	3.53	3.28	3.01	3.25	3.26	3.08	2.91	3.20	2.88	3.09	2.87
	H10-H15	2.10	1.83	1.51	1.66	1.67	1.58	1.41	1.66	1.32	1.52	1.29
	H12-H13	1.49	1.22	0.91	1.06	1.06	0.98	0.86	1.02	0.77	0.97	0.80
9	**H3-H5**	2.10	1.67	1.61	1.82	1.82	1.76	1.67	1.86	1.56	1.73	1.59
	H2-H6	1.64	1.18	1.09	1.28	1.27	1.26	1.11	1.34	0.98	1.21	1.00
	H8-H9	1.29	0.88	0.82	1.02	1.00	0.94	0.88	1.05	0.78	0.91	0.80
10	**H13**	3.97	3.58	3.19	3.49	3.50	3.38	3.21	3.46	3.15	3.41	3.19
	H12	2.51	2.39	1.99	2.22	2.24	2.13	2.02	2.18	1.93	2.09	1.91
	H$_3$C10	2.12	2.35	2.19	2.31	2.34	2.25	2.08	2.32	2.00	2.28	2.10
	H$_3$C11	1.11	0.96	0.82	0.88	0.89	0.86	0.73	0.88	0.70	0.84	0.68
11	**H10, H19**	3.76	3.27	2.88	3.17	3.19	3.07	3.00	3.12	2.83	3.09	2.86
	H$_3$C11, H$_3$C15	1.07	0.90	0.77	0.82	0.84	0.80	0.66	0.81	0.63	0.77	0.63
12	**H12, H13**	2.61	2.53	2.12	2.37	2.38	2.28	2.17	2.32	2.11	2.25	2.08
	H$_3$C10, H$_3$C11	2.21	2.46	2.31	2.44	2.46	2.37	2.20	2.42	2.16	2.40	2.23

Table S1, contd.

			M06-L									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**H6 e H9**	2.42	2.18	2.51	2.09	2.63	2.02	2.47	2.02	2.25	2.02	1.92
	H2 e H3	2.23	1.95	2.28	1.86	2.40	1.78	2.24	1.79	2.02	1.77	1.69
	H5 e H8	1.37	1.18	1.53	1.07	1.62	0.98	1.46	1.02	1.23	0.96	0.90
2	**H2-H4-H13-H14**	1.85	1.79	2.10	1.67	2.21	1.59	2.02	1.59	1.82	1.56	1.45
3	**H12-H13**	2.71	2.46	2.85	2.38	2.96	2.35	2.78	2.40	2.60	2.37	2.21
	H11-H14	1.71	1.56	1.92	1.41	2.01	1.36	1.83	1.41	1.63	1.39	1.24
4	**H3-H6-H8**	3.11	2.74	3.15	2.71	3.30	2.71	3.16	2.75	2.97	2.75	2.61
	H2-H5-H9	1.53	1.31	1.70	1.16	1.79	1.11	1.63	1.19	1.42	1.13	1.04
5	**H2-H4**	1.40	1.17	1.47	1.04	1.62	1.05	1.52	1.06	1.30	1.02	0.97
	C*H*$_3$	1.59	1.57	1.99	1.58	2.07	1.49	1.97	1.48	1.85	1.50	1.44
6	**H14**	3.96	3.64	3.18	3.53	4.11	3.51	3.93	3.48	3.19	3.52	3.37
	H12	3.46	3.16	2.71	3.10	3.64	3.05	3.49	3.04	2.78	3.06	2.93
	H10	3.44	2.95	2.46	2.85	3.39	2.82	3.20	2.82	2.45	2.86	2.62
	H15	2.34	1.93	1.39	1.80	2.37	1.79	2.17	1.81	1.47	1.76	1.55
	H13	1.92	1.50	1.01	1.44	1.98	1.39	1.81	1.43	1.11	1.38	1.22
	H11	1.56	1.13	0.63	1.04	1.60	1.00	1.40	1.05	0.69	0.99	0.79
7	**H14**	3.50	3.16	3.53	3.07	3.66	3.07	3.52	3.06	3.31	3.08	2.94
	H10	3.27	2.82	3.13	2.72	3.27	2.71	3.10	2.73	2.93	2.73	2.51
	H12	2.99	2.69	3.06	2.63	3.19	2.60	3.06	2.63	2.87	2.61	2.50
	H15	2.02	1.51	1.84	1.39	1.99	1.40	1.82	1.43	1.64	1.35	1.19
	H13	1.44	0.96	1.32	0.89	1.46	0.86	1.32	0.92	1.14	0.85	0.72
	H11	1.29	0.79	1.14	0.70	1.28	0.66	1.10	0.74	0.93	0.65	0.49
8	**H11-H14**	3.53	3.06	2.56	2.95	3.51	2.94	3.33	2.92	3.15	2.95	2.74
	H10-H15	2.10	1.57	1.05	1.45	2.02	1.47	1.85	1.49	1.69	1.43	1.22
	H12-H13	1.49	0.99	0.49	0.91	1.47	0.88	1.32	0.92	1.19	0.86	0.72
9	**H3-H5**	2.10	1.61	1.95	1.60	2.15	1.59	2.05	1.68	1.84	1.59	1.46
	H2-H6	1.64	1.14	1.46	1.12	1.66	1.13	1.53	1.24	1.40	1.11	0.92
	H8-H9	1.29	0.86	1.19	0.85	1.39	0.83	1.31	0.95	1.10	0.83	0.73
10	**H13**	3.97	3.42	2.30	3.21	2.57	3.28	2.42	3.23	3.52	3.35	3.13
	H12	2.51	2.08	3.60	1.99	3.84	1.95	3.70	1.96	2.26	1.94	1.80
	H$_3$C10	2.12	2.30	2.71	2.22	2.80	2.24	2.61	2.23	2.45	2.30	2.09
	H$_3$C11	1.11	0.93	1.37	0.88	1.44	0.88	1.29	0.89	1.22	0.89	0.74
11	**H10, H19**	3.76	3.15	3.33	2.99	3.57	3.02	3.43	3.00	3.23	3.10	2.90
	H$_3$C11, H$_3$C15	1.07	0.87	1.32	0.84	1.39	0.83	1.22	0.83	1.14	0.88	0.75
12	**H12, H13**	2.61	2.15	2.41	2.13	2.69	2.10	2.56	2.12	2.41	2.15	2.03
	H$_3$C10, H$_3$C11	2.21	2.42	2.82	2.35	2.89	2.34	2.71	2.32	2.57	2.42	2.24

Table S1, contd.

			PBE1PBE									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**H6 e H9**	2.42	2.42	2.23	2.22	2.34	2.13	2.02	2.20	1.87	2.16	2.01
	H2 e H3	2.23	2.14	1.95	1.94	2.05	1.83	1.74	1.91	1.60	1.86	1.73
	H5 e H8	1.37	1.27	1.09	1.05	1.17	0.93	0.84	1.01	0.69	0.95	0.82
2	**H2-H4-H13-H14**	1.85	1.93	1.64	1.68	1.81	1.58	1.46	1.66	1.30	1.60	1.43
3	**H12-H13**	2.71	2.79	2.49	2.54	2.66	2.47	2.33	2.52	2.17	2.49	2.31
	H11-H14	1.71	1.69	1.40	1.43	1.56	1.33	1.21	1.40	1.05	1.34	1.18
4	**H3-H6-H8**	3.11	3.18	2.89	2.99	3.09	2.92	2.82	2.98	2.65	2.96	2.80
	H2-H5-H9	1.53	1.38	1.12	1.16	1.29	1.04	0.97	1.13	0.81	1.04	0.94
5	**H2-H4**	1.40	1.25	0.91	1.00	1.13	0.91	0.86	0.97	0.68	0.95	0.85
	C*H*$_3$	1.59	1.69	1.47	1.52	1.63	1.49	1.42	1.54	1.32	1.49	1.42
6	**H14**	3.96	3.76	3.44	3.61	3.72	3.47	3.31	3.55	3.23	3.47	3.27
	H12	3.46	3.33	3.03	3.20	3.29	3.06	2.93	3.15	2.85	3.06	2.89
	H10	3.44	3.17	2.81	2.99	3.07	2.88	2.67	2.96	2.58	2.88	2.62
	H15	2.34	2.17	1.78	1.91	2.01	1.83	1.65	1.89	1.52	1.78	1.54
	H13	1.92	1.74	1.41	1.52	1.63	1.44	1.30	1.52	1.17	1.41	1.22
	H11	1.56	1.42	1.05	1.17	1.27	1.08	0.91	1.16	0.77	1.04	0.82
7	**H14**	3.50	3.35	3.04	3.19	3.30	3.09	2.96	3.18	2.84	3.09	2.91
	H10	3.27	3.08	2.74	2.91	2.98	2.81	2.63	2.89	2.52	2.81	2.58
	H12	2.99	2.92	2.63	2.78	2.87	2.67	2.56	2.76	2.45	2.67	2.52
	H15	2.02	1.72	1.38	1.47	1.59	1.41	1.26	1.48	1.13	1.34	1.14
	H13	1.44	1.17	0.86	0.95	1.06	0.88	0.77	0.96	0.63	0.83	0.69
	H11	1.29	1.00	0.68	0.77	0.88	0.68	0.55	0.77	0.40	0.63	0.45
8	**H11-H14**	3.53	3.17	2.82	3.00	3.10	2.89	2.71	2.96	2.61	2.88	2.65
	H10-H15	2.10	1.84	1.44	1.57	1.67	1.52	1.34	1.58	1.21	1.46	1.22
	H12-H13	1.49	1.19	0.81	0.95	1.04	0.87	0.76	0.92	0.64	0.86	0.68
9	**H3-H5**	2.10	1.74	1.43	1.90	1.69	1.55	1.45	1.64	1.30	1.52	1.37
	H2-H6	1.64	1.34	0.99	1.46	1.23	1.15	0.98	1.21	0.83	1.09	0.87
	H8-H9	1.29	1.04	0.71	1.19	0.96	0.83	0.76	0.93	0.62	0.80	0.68
10	**H13**	3.97	3.57	3.18	3.34	3.46	3.26	3.09	3.29	2.98	3.28	3.04
	H12	2.51	2.42	2.03	2.16	2.27	2.08	1.97	2.11	1.84	2.04	1.86
	H$_3$C10	2.12	2.43	2.26	2.28	2.39	2.23	2.04	2.28	1.94	2.26	2.05
	H$_3$C11	1.11	1.04	0.90	0.87	0.97	0.85	0.70	0.87	0.67	0.83	0.68
11	**H10, H19**	3.76	3.27	2.80	3.35	3.15	2.96	2.78	2.98	2.68	2.96	2.72
	H$_3$C11, H$_3$C15	1.07	0.98	0.76	1.11	0.91	0.79	0.63	0.80	0.59	0.76	0.60
12	**H12, H13**	2.61	2.56	2.07	2.29	2.41	2.22	2.12	2.25	2.03	2.20	2.02
	H$_3$C10, H$_3$C11	2.21	2.54	2.25	2.39	2.51	2.34	2.16	2.38	2.09	2.37	2.18

Table S1, contd.

			TPSSh									
	Atoms	Expt.	aug-cc-p-VDZ		aug-cc-p-VTZ		def2-TZVPP		pcSseg-2		x2c-TZVPPAll-s	
			GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
1	H6 e H9	2.42	2.38	2.18	2.28	2.31	2.18	2.08	2.26	1.94	2.20	2.06
	H2 e H3	2.23	2.14	1.95	2.05	2.07	1.93	1.85	2.01	1.72	1.96	1.84
	H5 e H8	1.37	1.28	1.08	1.16	1.19	1.03	0.95	1.12	0.81	1.04	0.93
2	H2-H4-H13-H14	1.85	1.90	1.69	1.76	1.80	1.65	1.54	1.73	1.39	1.67	1.50
3	H12-H13	2.71	2.77	2.55	2.63	2.65	2.53	2.41	2.60	2.27	2.56	2.38
	H11-H14	1.71	1.72	1.50	1.56	1.60	1.45	1.34	1.53	1.19	1.46	1.31
4	H3-H6-H8	3.11	3.12	2.90	3.02	3.04	2.94	2.85	3.02	2.70	2.98	2.83
	H2-H5-H9	1.53	1.44	1.25	1.33	1.36	1.19	1.13	1.29	0.98	1.19	1.09
5	H2-H4	1.40	1.26	0.99	1.12	1.17	1.03	0.98	1.08	0.82	1.06	0.96
	C*H*$_3$	1.59	1.64	1.52	1.57	1.59	1.53	1.47	1.58	1.37	1.31	1.46
6	H14	3.96	3.78	3.54	3.73	3.75	3.58	3.44	3.67	3.37	3.58	3.39
	H12	3.46	3.33	3.10	3.29	3.30	3.14	3.03	3.25	2.97	3.15	2.99
	H10	3.44	3.13	2.85	3.07	3.06	2.94	2.74	3.03	2.67	2.94	2.69
	H15	2.34	2.18	1.87	2.01	2.02	1.92	1.75	1.98	1.63	1.86	1.64
	H13	1.92	1.64	1.48	1.61	1.63	1.52	1.40	1.60	1.27	1.49	1.32
	H11	1.56	1.38	1.10	1.23	1.24	1.13	0.98	1.21	0.84	1.09	0.88
7	H14	3.50	3.34	3.11	3.28	3.30	3.16	3.05	3.27	2.95	3.17	3.00
	H10	3.27	3.02	2.76	2.95	2.95	2.84	2.68	2.94	2.58	2.85	2.62
	H12	2.99	2.88	2.67	2.84	2.84	2.72	2.63	2.83	2.52	2.72	2.58
	H15	2.02	1.75	1.49	1.60	1.62	1.53	1.39	1.59	1.26	1.45	1.26
	H13	1.44	1.19	0.96	1.07	1.09	0.98	0.89	1.07	0.76	0.94	0.80
	H11	1.29	1.00	0.76	0.87	0.89	0.77	0.65	0.86	0.52	0.72	0.55
8	H11-H14	3.53	3.18	2.91	3.11	3.13	2.99	2.82	3.08	2.74	2.98	2.77
	H10-H15	2.10	1.83	1.52	1.66	1.67	1.59	1.43	1.66	1.31	1.53	1.31
	H12-H13	1.49	1.23	0.93	1.08	1.09	1.00	0.89	1.05	0.78	0.98	0.82
9	H3-H5	2.10	1.81	1.57	1.75	1.76	1.69	1.61	1.79	1.46	1.67	1.52
	H2-H6	1.64	1.37	1.10	1.28	1.27	1.26	1.10	1.33	0.96	1.21	0.99
	H8-H9	1.29	1.06	0.81	0.99	0.99	0.93	0.87	1.04	0.75	0.90	0.80
10	H13	3.97	3.57	3.17	3.45	3.47	3.36	3.20	3.40	3.10	3.37	3.15
	H12	2.51	2.41	2.01	2.25	2.28	2.17	2.06	2.19	1.95	2.12	1.95
	C10H$_3$	2.12	2.38	2.22	2.33	2.35	2.27	2.09	2.32	2.00	2.30	2.11
	C11H$_3$	1.11	1.00	1.30	0.92	0.94	0.90	0.76	0.92	0.73	0.88	0.74
11	H10, H19	3.76	3.28	2.89	3.16	3.18	3.07	2.91	3.10	2.82	3.07	2.84
	H$_3$C11, H$_3$C15	1.07	0.95	0.82	0.87	0.88	0.85	0.70	0.86	0.66	0.82	0.67
12	H12, H13	2.61	2.54	2.13	2.38	2.40	2.30	2.20	2.34	2.13	2.26	2.10
	H$_3$C10, H$_3$C11	2.21	2.49	2.32	2.44	2.49	2.38	2.21	2.42	2.15	2.41	2.22

Table S2. Calculated ^{13}C-NMR chemical shifts of polyarsenicals **1-12** in chloroform by using combinations of methods (GIAO, CSGT), functionals (OLYP, M06-L, PBE1PBE, TPSSh) and the indicated basis sets; experimental values in $CDCl_3$ for comparison, in redline. For the numbering of H and C atoms, see structures in Figure S1.

			OLYP									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**C4 e C7**	23.05	28.32	25.98	27.26	26.74	25.50	22.65	27.16	26.46	25.55	24.88
	C1	17.03	26.44	23.79	24.82	24.24	23.15	20.74	24.51	24.02	23.00	22.54
2	**C1-C3**	30.60	33.62	31.73	33.34	32.74	31.72	28.40	33.50	32.57	31.79	30.87
3	**C1-C3**	23.71	30.36	28.51	29.61	29.21	28.10	25.26	29.80	29.01	28.16	27.33
4	**C1-C4-C7**	17.82	27.41	24.83	25.88	28.91	24.43	21.95	26.08	25.39	24.52	23.84
5	**C1-C3**	32.32	36.07	33.75	34.97	34.80	34.63	31.72	35.74	35.10	34,23	33.83
	CH$_3$	10.29	11.46	13.39	12.35	13.04	11.71	11.47	12.61	12.38	12.83	12.49
6	**C9**	42.20	53.47	50.39	52.28	52.01	51.38	48.72	53.79	53.20	50.86	49.91
	C7	27.40	39.60	36.79	38.15	37.79	37.06	34.64	38.99	38.50	36.49	35.81
	C2	25.70	37.12	34.28	35.55	35.07	34.15	31.52	36.09	35.61	33.39	32.51
7	**C9**	45.14	53.10	50.26	52.25	52.00	51.34	48.61	53.86	53.27	50.99	50.18
	C2	33.58	42.46	39.89	41.60	41.21	40.30	37.62	42.60	42.05	39.86	39.08
	C7	31.40	40.61	37.87	39.48	39.14	38.49	36.00	40.48	39.93	38.06	37.46
8	**C2-C9**	38.90	49.26	46.35	48.03	47.75	46.89	47.96	49.34	48.70	46.35	45.39
	C8	8.10	19.76	16.83	16.71	16.43	15.91	17.71	16.75	16.53	15.11	14.44
9	**C1-C4**	45.3	53.60	53.90	52.69	52.48	52.46	49.93	54.85	54.30	52.05	51.21
	C7	32.5	42.57	42.95	41.43	41.17	41.14	38.82	43.06	42.66	40.61	40.06
10	**C7**	48.8	57.40	59.07	56.56	56.18	56.56	54.08	58.43	58.14	55.42	54.85
	C1	43.0	53.43	54.78	52.40	51.90	52.34	49.94	53.87	53.71	51.14	50.70
	C11	20.0	18.96	25.87	20.60	21.57	20.22	19.90	21.60	21.27	21.71	21.18
	C10	13.3	12.58	19.38	13.84	14.88	13.74	13.56	14.57	14.16	14.88	14.39
11	**C1, C7**	48.8	57.08	54.11	56.21	55.75	56.23	53.77	57.88	57.79	54.99	54.48
	C11, C15	19.8	18.68	21.08	20.35	21.37	20.00	19.69	21.48	21.18	21.47	20.96
12	**C1, C7**	42.5	53.17	49.88	52.12	51.61	51.97	49.58	53.40	53.44	50.86	50.39
	C10, C11	12.9	12.55	14.68	13.82	14.76	13.66	13.53	14.63	14.33	14.76	14.32

Table S2, contd.

			M06-L									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**C4 e C7**	23.05	23.50	22.58	19.93	21.81	20.57	19.59	20.75	21.26	19.04	18.91
	C1	17.03	21.58	20.60	17.62	19.37	18.11	17.57	18.12	18.81	16.40	16.41
2	**C1-C3**	30.60	28.24	27.68	25.51	27.23	26.30	24.79	24.50	31.07	24.60	24.35
3	**C1-C3**	23.71	25.46	24.71	19.11	23.83	22.53	20.71	23.15	23.83	21.43	20.84
4	**C1-C4-C7**	17.82	23.72	21.87	16.96	20.87	19.37	19.11	19.98	20.73	18.46	17.99
5	**C1-C3**	32.32	33.40	32.42	28.93	31.51	31.11	30.30	31.69	32.44	29.54	29.88
	***C*H3**	10.29	14.81	17.54	16.26	16.71	14.32	16.23	14.66	16.76	14.41	14.93
6	**C9**	42.20	49.03	47.13	43.20	45.99	45.65	45.25	46.48	44.54	43.66	43.34
	C7	27.40	36.08	34.31	30.15	32.83	32.17	31.88	32.92	31.34	30.31	29.92
	C2	25.70	33.26	31.91	27.01	30.29	39.39	29.04	30.16	28.73	27.56	27.00
7	**C9**	45.14	47.69	46.18	42.37	45.34	44.97	44.41	45.99	47.03	43.13	42.83
	C2	33.58	37.58	36.36	31.69	35.27	34.44	34.00	35.46	36.40	32.90	32.37
	C7	31.40	35.81	34.49	30.30	33.48	32.75	32.37	33.75	34.64	31.12	30.68
8	**C2-C9**	38.90	45.01	43.13	38.86	41.89	41.51	41.00	42.26	43.20	39.62	39.09
	C8	8.10	16.69	14.66	10.24	12.53	11.43	11.37	11.51	12.46	9.62	9.27
9	**C1-C4**	45.3	49.59	47.7	44.70	46.9	46.96	46.6	48.17	49.2	45.07	44.61
	C7	32.5	39.04	37.3	34.11	36.3	36.18	36.0	37.32	38.1	34.34	33.96
10	**C7**	48.8	54.78	52.67	48.33	51.46	51.56	51.82	52.99	53.98	49.81	49.70
	C1	43.0	51.37	49.55	45.36	48.18	48.34	48.64	49.49	50.77	46.14	46.42
	C11	20.0	22.45	24.79	21.36	24.26	22.38	23.95	22.59	24.63	22.44	22.93
	C10	13.3	17.27	19.24	13.45	18.62	16.46	18.37	16.92	18.71	16.85	16.95
11	**C1, C7**	48.8	51.96	52.48	48.11	51.30	51.50	51.68	53.09	53.81	54.00	54.04
	C11, C15	19.8	20.28	24.64	22.36	24.08	22.08	23.76	22.93	24.41	25.14	25.76
12	**C1, C7**	42.5	51.77	49.13	45.91	47.71	48.32	48.12	49.24	50.29	49.89	50.27
	C10, C11	12.9	16.72	19.17	15.31	18.52	16.23	18.32	17.36	18.64	19.80	19.99

Table S2, contd.

			PBE1PBE									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**C4 e C7**	23.05	28.13	25.80	26.25	26.39	25.58	22.52	26.23	25.39	24.87	24.45
	C1	17.03	25.12	22.52	22.68	22.78	21.96	19.37	22.41	21.77	21.06	20.85
2	**C1-C3**	30.60	34.34	32.36	33.14	33.21	32.72	29.15	32.61	32.32	31.98	31.33
3	**C1-C3**	23.71	29.98	28.03	28.36	28.57	27.91	26.99	28.51	27.59	27.14	26.57
4	**C1-C4-C7**	17.82	26.46	23.73	24.01	24.29	23.43	20.81	24.07	23.29	22.74	22.35
5	**C1-C3**	32.32	36.84	34.38	34.97	35.34	35.05	32.21	35.58	34.78	34.18	34.15
	$\underline{C}H_3$	10.29	10.76	12.63	11.23	12.41	10.58	10.43	11.20	11.11	11.21	11.38
6	**C9**	42.20	52.19	49.10	50.17	50.51	50.01	47.23	51.31	50.51	48.78	48.15
	C7	27.40	38.27	35.49	36.06	36.27	35.69	33.13	36.71	36.02	34.41	33.97
	C2	25.70	36.55	33.72	34.28	34.36	33.64	30.84	34.69	33.95	32.21	31.50
7	**C9**	45.14	52.10	49.24	50.47	50.80	50.34	48.87	51.73	50.97	49.33	48.80
	C2	33.58	43.13	39.55	40.53	40.71	40.06	38.59	41.35	40.59	38.99	38.38
	C7	31.40	39.53	36.83	37.64	37.90	37.42	36.19	38.48	37.79	36.33	35.97
8	**C2-C9**	38.90	48.16	45.25	46.18	46.47	45.82	42.96	47.13	46.28	44.60	43.89
	C8	8.10	17.97	15.05	14.26	14.51	13.94	11.74	14.08	13.73	12.41	11.99
9	**C1-C4**	45.3	53.38	50.29	51.77	52.11	52.00	49.40	53.52	52.78	51.06	50.47
	C7	32.5	41.93	38.94	40.03	40.36	40.27	37.93	41.44	40.89	39.17	38.89
10	**C7**	48.8	57.01	53.94	55.44	55.62	55.59	53.26	56.75	56.21	54.10	53.80
	C1	43.0	52.30	48.94	50.42	50.49	50.56	48.44	51.40	51.29	48.91	48.91
	C11	20.0	19.28	21.41	20.45	21.87	20.14	19.90	21.00	20.92	21.10	21.20
	C10	13.3	12.41	14.43	13.17	14.61	12.93	12.80	13.44	13.19	13.56	13.59
11	**C1, C7**	48.8	56.71	53.63	55.18	55.28	55.31	53.03	56.31	56.10	53.73	53.51
	C11, C15	19.8	19.05	21.24	20.23	21.70	19.95	19.71	20.93	20.93	20.89	20.99
12	**C1, C7**	42.5	51.95	48.54	50.03	50.09	50.10	47.97	50.86	51.06	48.51	48.48
	C10, C11	12.9	12.37	14.29	13.07	14.46	12.81	12.73	13.48	13.41	13.41	13.48

Table S2, contd.

			TPSSh									
	Atoms	**Expt.**	**aug-cc-p-VDZ**		**aug-cc-p-VTZ**		**def2-TZVPP**		**pcSseg-2**		**x2c-TZVPPAll-s**	
			GIAO	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**	**GIAO**	**CSGT**
1	**C4 e C7**	23.05	26.72	24.46	25.42	24.93	24.72	21.74	25.42	24.61	23.97	23.53
	C1	17.03	24.26	21.72	22.44	21.88	21.74	19.21	22.21	21.60	20.79	20.53
2	**C1-C3**	30.60	32.50	30.59	31.85	31.30	31.36	27.87	32.11	31.07	30.57	29.91
3	**C1-C3**	23.71	28.63	26.80	27.60	27.22	27.14	24.17	27.82	26.95	26.33	25.76
4	**C1-C4-C7**	17.82	25.50	22.84	23.55	23.31	23.11	20.53	23.78	23.02	22.36	21.93
5	**C1-C3**	32.32	35.73	33.56	34.52	34.35	34.66	31.91	35.28	34.50	33.66	33.58
	$\underline{C}H_3$	10.29	11.68	13.60	12.89	13.45	12.28	12.14	12.90	12.81	12.95	13.06
6	**C9**	42.20	52.04	49.05	50.55	50.29	50.48	47.80	51.90	51.15	49.20	48.58
	C7	27.40	37.93	35.25	36.32	35.92	36.03	33.57	37.11	36.49	34.73	34.27
	C2	25.70	35.70	33.02	34.06	33.55	33.50	30.84	34.59	33.96	32.04	31.36
7	**C9**	45.14	51.63	48.89	50.53	50.26	50.46	47.68	51.97	51.25	49.39	48.85
	C2	33.58	41.01	38.58	40.01	39.59	39.58	36.84	40.95	40.27	38.46	37.86
	C7	31.40	38.85	36.27	37.57	37.31	37.40	34.85	38.53	37.88	36.27	35.86
8	**C2-C9**	38.90	47.84	45.04	46.37	46.08	46.10	43.36	47.53	46.75	44.85	44.15
	C8	8.10	17.66	14.83	14.59	14.29	14.42	12.33	14.58	14.26	12.92	12.46
9	**C1-C4**	45.3	53.05	50.16	52.01	51.79	52.32	49.81	53.96	53.27	51.31	50.70
	C7	32.5	41.52	38.73	40.27	40.03	40.61	38.30	41.86	41.33	39.44	39.10
10	**C7**	48.8	56.20	54.02	55.76	55.42	56.11	53.91	57.38	56.90	54.41	54.10
	C1	43.0	52.01	49.46	51.31	50.83	51.64	49.60	52.59	52.48	49.77	49.73
	C11	20.0	18.98	21.84	21.40	22.33	21.24	21.02	22.14	22.04	22.22	22.26
	C10	13.3	12.51	15.28	14.61	15.55	14.53	14.43	15.03	14.80	15.22	15.22
11	**C1, C7**	48.8	56.61	53.78	55.59	55.13	55.90	53.73	57.19	56.99	54.10	53.87
	C11, C15	19.8	19.39	21.67	21.24	22.16	21.06	20.84	22.25	22.20	22.02	22.06
12	**C1, C7**	42.5	52.23	48.99	50.92	50.38	51.12	49.08	52.18	52.33	49.33	49.25
	C10, C11	12.9	13.10	15.13	14.55	15.41	14.42	14.37	15.26	15.16	15.07	15.10

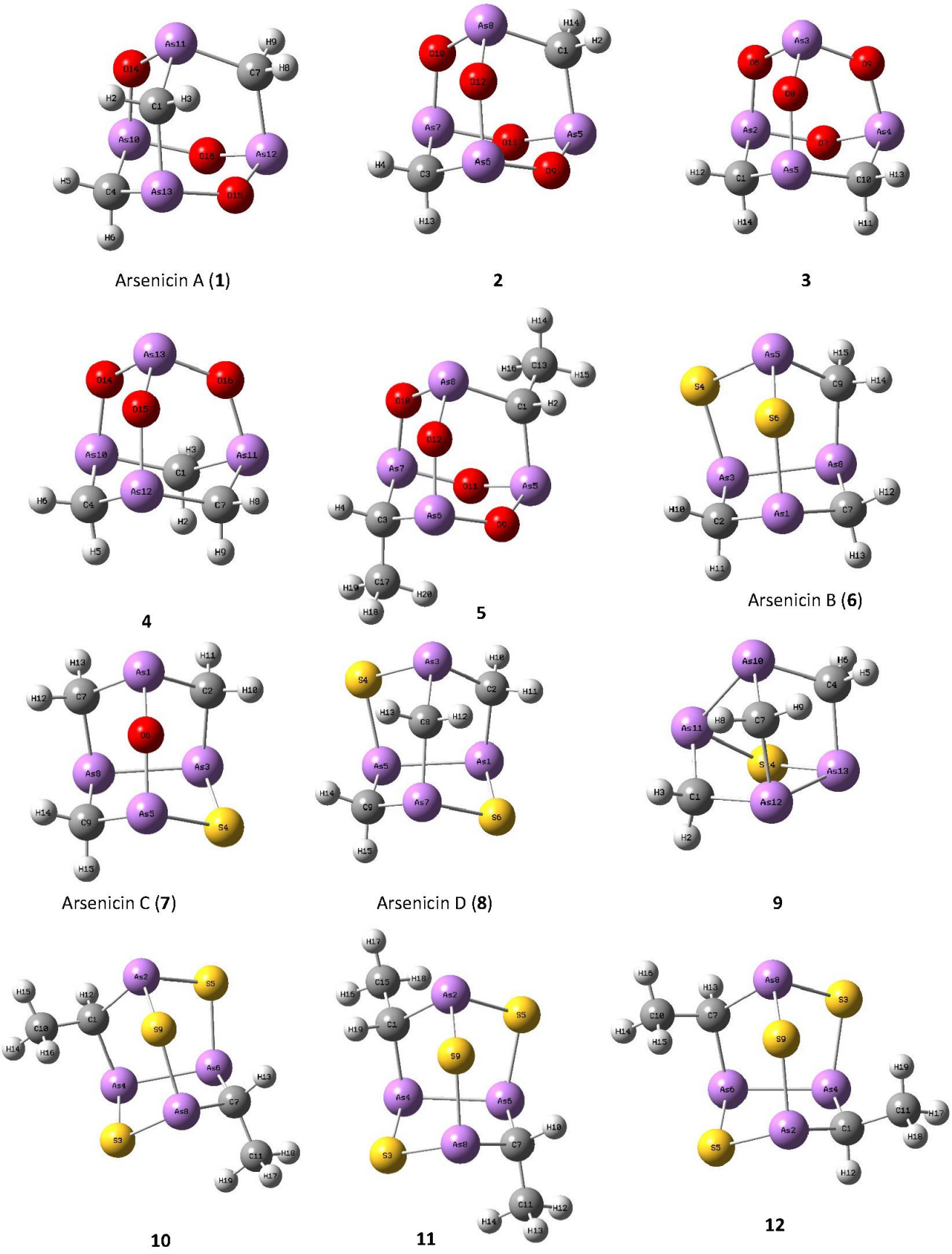

Figure S1. Molecular structures (energy minimized using C-PCM in chloroform, B1B95/6-311+G(3df,2pd) of polyarsenicals **1**-**12** evaluated in the NMR calculations.

Table S3. xyz Coordinates of geometry optimized structures of compounds **1**-**12**.

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Arsenicin A (**1**)

C	0.00000	0.00000	-2.11395
H	-0.58715	0.65000	-2.76166
H	0.58715	-0.65000	-2.76166
C	0.00000	2.08822	0.00450
H	-0.63726	2.69567	-0.63857
H	0.57605	2.76996	0.62789
C	0.00000	-2.08822	0.00450
H	0.63726	-2.69567	-0.63857
H	-0.57605	-2.76996	0.62789
As	-1.19429	1.09604	1.19553
As	-1.26429	-1.14870	-1.15950
As	1.19429	-1.09604	1.19553
As	1.26429	1.14870	-1.15950
O	-1.97676	0.02490	0.00994
O	1.97676	-0.02490	0.00994
O	0.00000	0.00000	1.95466

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COMPOUND **2**

C	0.00000	-2.06517	0.00000
H	-0.62210	-2.70786	0.62210
C	0.00000	2.06517	0.00000
H	0.62210	2.70786	0.62210
As	-1.19861	-1.08662	-1.19862
As	-1.19861	1.08662	1.19862
As	1.19861	1.08662	-1.19862
As	1.19861	-1.08662	1.19862
O	-1.95987	0.00000	0.00000
O	1.95987	0.00000	0.00000
O	0.00000	0.00000	-1.95987
O	0.00000	0.00000	1.95987
H	-0.62210	2.70786	-0.62210
H	0.62210	-2.70786	-0.62210

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COMPOUND **3**

C	0.86176	-1.48452	-1.20073
As	-1.00799	-1.61647	-0.64833
As	-0.01971	-0.00113	1.96165
As	-1.00819	1.61710	-0.64648
As	1.97899	0.00049	-0.58318
O	-0.79925	-1.35789	1.11458
O	-1.57536	0.00057	-1.15826
O	1.56274	-0.00061	1.17867
O	-0.79937	1.35653	1.11612
C	0.86145	1.48588	-1.19930
H	0.86417	1.46062	-2.28912
H	1.34987	-2.40870	-0.89587
H	1.34952	2.40989	-0.89383
H	0.86475	-1.45840	-2.29052

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COMPOUND **4**

C	1.48723	0.85865	-1.23033
H	1.41373	0.81622	-2.31782
H	2.40600	1.38910	-0.99151
C	-1.48723	0.85865	-1.23033
H	-1.41373	0.81622	-2.31782
H	-2.40600	1.38910	-0.99151
C	0.00000	-1.71730	-1.23033
H	0.00000	-2.77820	-0.99151
H	0.00000	-1.63244	-2.31782
As	0.00000	1.97116	-0.61049
As	1.70708	-0.98558	-0.61049
As	-1.70708	-0.98558	-0.61049
As	0.00000	0.00000	1.96402
O	0.00000	1.57476	1.15415
O	-1.36378	-0.78738	1.15415
O	1.36378	-0.78738	1.15415

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COMPOUND **5**

C	0.00000	2.09141	0.05709
H	0.65385	2.67939	0.70344
C	0.00000	-2.09141	0.05709
H	-0.65385	-2.67939	0.70344
As	1.20931	1.07256	-1.11037
As	1.18022	-1.10359	1.27959
As	-1.20931	-1.07256	-1.11037
As	-1.18022	1.10359	1.27959
O	1.95917	-0.02025	0.08901
O	-1.95917	0.02025	0.08901
O	0.00000	0.00000	-1.87787
O	0.00000	0.00000	2.04135
C	-0.85959	3.00142	-0.81319
H	-1.48796	3.65496	-0.20867
H	-0.24727	3.63946	-1.44989
H	-1.51242	2.41616	-1.45848
C	0.85959	-3.00142	-0.81319
H	1.48796	-3.65496	-0.20867
H	0.24727	-3.63946	-1.44989
H	1.51242	-2.41616	-1.45848

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Arsenicin B (**6**)

As	-1.79614	1.22764	-0.30163
C	-1.41396	-0.21995	-1.55826
As	-0.16841	-1.64653	-1.00966
S	1.79646	-0.62379	-1.32885
As	1.89658	0.95103	0.24526
S	0.16746	2.30761	-0.17294
C	-1.74887	0.11742	1.30817
As	-0.38164	-1.28949	1.41496
C	1.19707	-0.15396	1.69780
H	-1.05271	0.19600	-2.49530
H	-2.37049	-0.70471	-1.75140
H	-1.63847	0.76617	2.17428
H	-2.72138	-0.36617	1.37623
H	0.97455	0.50540	2.53612
H	2.01711	-0.80649	1.98797

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Arsenicin C (**7**)

As	-1.48598	1.42222	-0.46585
C	-1.27010	-0.12908	-1.63152
As	-0.14501	-1.59893	-0.95513
S	1.85429	-0.61156	-1.17845
As	1.72350	1.07600	0.27878
O	0.22724	1.91609	-0.20599
C	-1.79387	0.35084	1.13681
As	-0.52922	-1.12412	1.43301
C	1.05411	-0.00909	1.75690
H	-0.86501	0.17910	-2.59231
H	-2.27034	-0.52873	-1.79936
H	-1.76658	0.99903	2.01065
H	-2.79838	-0.06137	1.06026
H	0.81026	0.66111	2.58160
H	1.87426	-0.64929	2.07216

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Arsenicin D (**8**)

As	-0.27434	-1.44051	1.20416
C	1.03296	-0.10218	1.81270
As	1.66984	1.26157	0.56924
S	2.09142	-0.14799	-1.10986
As	0.27434	-1.44052	-1.20416
S	-2.09142	-0.14799	1.10986
As	-1.66984	1.26157	-0.56924
C	0.00000	2.12292	0.00000
C	-1.03296	-0.10218	-1.81270
H	1.91593	-0.64240	2.14638
H	0.58315	0.38475	2.67704
H	-0.28542	2.77501	0.82494
H	0.28542	2.77502	-0.82494
H	-0.58315	0.38474	-2.67705
H	-1.91593	-0.64240	-2.14638

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COMPOUND **9**

C	0.00000	0.00000	-2.07563
H	-0.44596	0.76172	-2.71178
H	0.44596	-0.76172	-2.71178
C	0.00000	1.98162	-0.11090
H	-0.42938	2.61148	-0.89035
H	0.43086	2.61656	0.65814
C	0.00000	-1.98162	-0.11090
H	0.42938	-2.61148	-0.89035
H	-0.43086	-2.61656	0.65814
As	1.36699	0.87661	-0.97340
As	-1.42028	0.92219	0.74043
As	-1.36699	-0.87661	-0.97340
As	1.42028	-0.92219	0.74043
S	0.00000	0.00000	2.19055

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COMPOUND **10**

C	1.81299	0.02581	1.14406
As	2.10881	-0.17973	-0.79000
S	-1.18438	-1.19652	1.62314
As	0.04607	0.65717	1.79126
S	1.11312	1.70332	-1.42867
As	-0.77163	1.79438	-0.23184
C	-1.82961	0.32687	-1.03461
As	-1.39739	-1.53430	-0.57234
S	0.68868	-1.81934	-1.34080
C	2.25520	-1.22070	1.89644
C	-3.29128	0.55770	-0.66948
H	2.46471	0.86723	1.38550
H	-1.66748	0.41685	-2.10842
H	2.18376	-1.07387	2.97286
H	3.28969	-1.46834	1.66479
H	1.63172	-2.07114	1.63172
H	-3.93770	-0.18446	-1.13690
H	-3.62092	1.54203	-0.99797
H	-3.43973	0.49635	0.40751

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COMPOUND **11**

C	-1.77894	-0.12759	1.17095
As	-1.86316	1.21242	-0.26437
S	1.40609	-0.18535	1.94051
As	-0.28941	-1.43075	1.19859
S	-1.40610	-0.18535	-1.94051
As	0.28941	-1.43075	-1.19859
C	1.77894	-0.12759	-1.17095
As	1.86316	1.21242	0.26437
S	0.00000	2.42209	0.00000
H	1.68088	0.43276	-2.10039
C	3.08127	-0.91814	-1.13127
H	3.14050	-1.60832	-1.97131
H	3.94621	-0.25737	-1.17990
H	3.15852	-1.49899	-0.21342
C	-3.08127	-0.91814	1.13127
H	-3.14050	-1.60832	1.97131
H	-3.94621	-0.25736	1.17990
H	-3.15852	-1.49899	0.21342
H	-1.68088	0.43276	2.10039

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COMPOUND **12**

C	-2.05471	-0.54070	-0.21426
As	-1.66325	0.88409	1.08470
S	0.70169	-2.29496	-0.34354
As	-0.67719	-1.02394	-1.55911
S	-0.70169	2.29496	-0.34350
As	0.67721	1.02397	-1.55908
C	2.05471	0.54070	-0.21423
As	1.66324	-0.88411	1.08470
S	-0.00002	-0.00002	2.30083
C	2.59789	1.78011	0.48123
C	-2.59790	-1.78012	0.48116
H	-2.82969	-0.07962	-0.82887
H	2.82970	0.07963	-0.82883
H	2.90395	2.53321	-0.24313
H	1.84235	2.22245	1.12570
H	3.46668	1.53441	1.08950
H	-2.90395	-2.53321	-0.24322
H	-3.46670	-1.53443	1.08943
H	-1.84237	-2.22248	1.12563

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