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Electronic Supporting Information

Proline *cis-trans* isomerization and its implications for the dimerization of analogues of cyclopeptide stylostatin 1: a combined computational and experimental study

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Table S1. NOE signals between peptide NH protons from ^{1}H-^{1}H NOESY 2D spectrum (Figure 4) for both conformers: *trans* c(KSTAIPF) (top) and *cis* c(KSTAIPF) (bottom).

trans c(KSTAIPF), major conformation in NMR experiments (green labels and circles in Figure 4)

Source NH proton	Vicinal interesting NH protons	Non-vicinal interesting NH protons (green circles)
Lys	Phe, Ser	Ile (weak)
Ser	Lys	Ala (weak), Ile
Thr	Ala, Ser (weak)	Ile
Ala	Ile, Thr	Ser
Ile	Ala	Thr, Ser, Lys (weak)
Pro	-	-
Phe	Lys	

cis c(KSTAIPF), minor conformation in NMR experiments (purple labels and circles in Figure 4)

Source NH proton	*Vicinal interesting NH protons*	*Non-vicinal interesting NH protons (purple circles)*
Lys	Phe, Ser	Ala
Ser	Thr	Ile (weak)
Thr	Ser	-
Ala	-	Phe
Ile	-	-
Pro	-	-
Phe	Lys	Ala

Table S2. Distances of β- and γ-turns in *cis* and *trans* cyclopeptides.[a]

Isomer	*Type*	*Residues* [a]	*c(NSLAIPF)*	*c(NSTAIPF)*	*c(KSTAIPF)*	*c(RSTAIPF)*	*c(DSTAIPF)*
Cis	β-turn (I)	$\mathbf{X^1}_i$-S^2_{i+1}-T^3_{i+2}-$\mathbf{A^4}_{i+3}$	3.4±0.4	3.3±0.4	3.2±0.3	3.2±0.4	3.3±0.4
Cis	β-turn (VIa1)	$\mathbf{A^4}_i$-I^5_{i+1}-P^6_{i+2}-$\mathbf{F^7}_{i+3}$	3.3±0.3	3.2±0.3	3.2±0.3	3.2±0.3	3.2±0.3
Trans	β-turn (II)	$\mathbf{S^2}_i$-X^3_{i+1}-A^4_{i+2}-$\mathbf{I^5}_{i+3}$	3.5±0.4	3.7±0.4	3.7±0.4	3.6±0.4	3.6±0.4
Trans	γ-turn	$\mathbf{F^7}_i$-X^1_{i+1}-$\mathbf{S^2}_{i+2}$	3.0±0.3	3.0±0.2	2.9±0.2	2.9±0.2	3.0±0.2
Trans	γ-turn	$\mathbf{I^5}_i$-P^6_{i+1}-$\mathbf{F^7}_{i+2}$	3.1±0.2	3.1±0.2	3.1±0.2	3.1±0.2	3.1±0.2

[a] Distance from carbonyl oxygen of residue i and the nitrogen of NH unit of residue i+2 (γ-turn) and i+3 (β-turn), shown in bold.

Table S3. Number of conformations selected (at least of 75 % of the conformational space covered) from 100 ns MD simulations for the *cis* and *trans* isomers of each cyclopeptide in order to compute by semiempirical and DFT methods the relative Gibbs free energies between both isomers. 256 conformations in total.

Cyclopeptides	*Cis isomer*	*Trans isomer*
c(NSLAIPF)	27	26
c(NSTAIPF)	25	25
c(KSTAIPF)	25	25
c(RSTAIPF)	24	27
c(DSTAIPF)	26	26

Table S4. Relative energies of *cis* conformers versus *trans* conformers for all studied cyclopeptides, in kcal/mol.[a]

Cyclopeptide	No. conf.	PM6-DH+	M06-2X/6-31G(d)	No. of conf.	M06-2X/6-31G(d,p)	M062X/def2-TZVP	MP2/6-31G(d)
Type of calculation	-	Geometry optimization and Frequency calculation	Geometry optimization and Frequency calculation	-	Geometry Optimization	Single point at M06-2X/6-31G(d) geometry	Single point at M06-2X/6-31G(d) geometry
c(NSLAIPF)	53	-7.5	-7.6	10	-6.7	-5.1	-4.1
c(NSTAIPF)	50	-8.2	-6.0	16	-4.9	-4.7	-4.7
c(KSTAIPF)	50	-2.6	-4.8	17	-3.5	-4.1	-3.0
c(RSTAIPF)	51	-3.6	-5.7	12	-5.5	-4.9	-4.0
c(DSTAIPF)	52	-9.4	-13.5	12	-13.1	-9.4	-8.4

Table S5. Gibbs free energy calculated at M06-2X/6-31G(d)/SMD level for all selected conformations for all studied cyclopeptides (conformation number, Gibbs free energy in hartree and % population according to the Boltzmann distribution)

cis c(NSLAIPF)

1	-2517.790747	5.03
2	-2517.787445	0.15
3	-2517.791012	6.66
4	-2517.789223	1.00
5	-2517.789382	1.19
6	-2517.789865	1.98
7	-2517.779866	0.00
8	-2517.785222	0.01
9	-2517.787730	0.21
10	-2517.785261	0.02
11	-2517.788020	0.28
12	-2517.792500	32.16
13	-2517.782317	0.00
14	-2517.787459	0.15
15	-2517.784863	0.01
16	-2517.788794	0.64
17	-2517.779962	0.00
18	-2517.788166	0.33
19	-2517.779621	0.00
20	-2517.792566	34.49
21	-2517.783774	0.00
22	-2517.778936	0.00
23	-2517.787933	0.26
24	-2517.790708	4.82
25	-2517.791390	9.93
26	-2517.788844	0.67
27	-2517.785614	0.02

trans c(NSLAIPF)

1	-2517.7679	0.00
2	-2517.7799	19.60
3	-2517.7675	0.00
4	-2517.7739	0.03
5	-2517.7680	0.00
6	-2517.7729	0.01
7	-2517.7798	16.97
8	-2517.7725	0.01
9	-2517.7687	0.00
10	-2517.7707	0.00
11	-2517.7681	0.00
12	-2517.7698	0.00
13	-2517.7710	0.00
14	-2517.7745	0.06
15	-2517.7709	0.00
16	-2517.7698	0.00
17	-2517.7793	10.06
18	-2517.7674	0.00
19	-2517.7684	0.00
20	-2517.7801	23.19
21	-2517.7803	30.05
22	-2517.7725	0.01
23	-2517.7690	0.00
24	-2517.7722	0.01
25	-2517.7689	0.00
26	-2517.7697	0.00

cis c(NSTAIPF)

1	-2514.451453	37.03
2	-2514.443638	0.01
3	-2514.449213	3.46
4	-2514.449448	4.43
5	-2514.444420	0.02
6	-2514.449499	4.68
7	-2514.450100	8.84
8	-2514.449431	4.35
9	-2514.445953	0.11
10	-2514.450016	8.09
11	-2514.445845	0.10
12	-2514.446974	0.32
13	-2514.440765	0.00
14	-2514.446339	0.16
15	-2514.441116	0.00
16	-2514.443736	0.01
17	-2514.441644	0.00
18	-2514.446806	0.27
19	-2514.443759	0.01
20	-2514.448427	1.50
21	-2514.442741	0.00
22	-2514.450692	16.55
23	-2514.446396	0.18
24	-2514.450203	9.86
25	-2514.443174	0.01

trans c(NSTAIPF)

1	-2514.429801	0.00
2	-2514.440731	10.07
3	-2514.426918	0.00
4	-2514.433761	0.01
5	-2514.428539	0.00

6	-2514.434732	0.02
7	-2514.436430	0.11
8	-2514.434313	0.01
9	-2514.431928	0.00
10	-2514.432552	0.00
11	-2514.431414	0.00
12	-2514.434409	0.01
13	-2514.441924	35.61
14	-2514.432565	0.00
15	-2514.441947	36.49
16	-2514.439544	2.87
17	-2514.431999	0.00
18	-2514.439910	4.22
19	-2514.435935	0.06
20	-2514.430548	0.00
21	-2514.439342	2.31
22	-2514.430346	0.00
23	-2514.430028	0.00
24	-2514.436931	0.18
25	-2514.440515	8.01

cis c(KSTAIPF)

1	-2519.382019	8.49
2	-2519.380661	2.02
3	-2519.381870	7.25
4	-2519.371864	0.00
5	-2519.381926	7.69
6	-2519.380675	2.05
7	-2519.378004	0.12
8	-2519.377611	0.08
9	-2519.382923	22.11
10	-2519.379780	0.79
11	-2519.380354	1.46
12	-2519.377236	0.05
13	-2519.379668	0.70
14	-2519.377388	0.06
15	-2519.373092	0.00
16	-2519.374982	0.00
17	-2519.381143	3.36
18	-2519.378940	0.33
19	-2519.371389	0.00
20	-2519.379496	0.59
21	-2519.380443	1.60
22	-2519.373845	0.00
23	-2519.382330	11.80
24	-2519.382683	17.15
25	-2519.382368	12.29

trans c(KSTAIPF)

1	-2519.370764	0.18
2	-2519.375702	33.03
3	-2519.374916	14.37
4	-2519.375363	23.07
5	-2519.366778	0.00
6	-2519.362092	0.00
7	-2519.366615	0.00
8	-2519.368785	0.02
9	-2519.369223	0.03
10	-2519.363730	0.00
11	-2519.372449	1.06
12	-2519.367274	0.00
13	-2519.372496	1.11
14	-2519.364745	0.00
15	-2519.368020	0.01
16	-2519.374571	9.97
17	-2519.367816	0.01
18	-2519.365115	0.00
19	-2519.366853	0.00
20	-2519.365665	0.00
21	-2519.361614	0.00
22	-2519.370321	0.11
23	-2519.375074	16.99
24	-2519.369042	0.03
25	-2519.364152	0.00

cis c(RSTAIPF)

1	-2628.870030	32.50
2	-2628.861425	0.00
3	-2628.867061	1.40
4	-2628.862155	0.01
5	-2628.866494	0.77
6	-2628.867628	2.56
7	-2628.863937	0.05
8	-2628.865379	0.24
9	-2628.868941	10.26
10	-2628.870080	34.27
11	-2628.865162	0.19
12	-2628.863874	0.05
13	-2628.863233	0.02
14	-2628.867210	1.64
15	-2628.861648	0.00
16	-2628.868518	6.56
17	-2628.863232	0.02
18	-2628.867846	3.22
19	-2628.868398	5.77
20	-2628.860010	0.00
21	-2628.864761	0.12
22	-2628.864945	0.15

23	-2628.864435	0.09
24	-2628.864617	0.11

trans c(RSTAIPF)

1	-2628.851926	0.00
2	-2628.859905	11.15
3	-2628.861556	64.02
4	-2628.860539	21.81
5	-2628.851662	0.00
6	-2628.848352	0.00
7	-2628.851327	0.00
8	-2628.849003	0.00
9	-2628.853836	0.02
10	-2628.853441	0.01
11	-2628.852480	0.00
12	-2628.854747	0.05
13	-2628.852524	0.00
14	-2628.849822	0.00
15	-2628.850511	0.00
16	-2628.846776	0.00
17	-2628.850750	0.00
18	-2628.856342	0.26
19	-2628.857366	0.76
20	-2628.852866	0.01
21	-2628.856802	0.42
22	-2628.853848	0.02
23	-2628.857961	1.42
24	-2628.854324	0.03
25	-2628.853687	0.02
26	-2628.851359	0.00
27	-2628.846537	0.00

cis c(DSTAIPF)

1	-2533.882273	49.17
2	-2533.873707	0.01
3	-2533.877589	0.35
4	-2533.879597	2.89
5	-2533.880074	4.79
6	-2533.877057	0.20
7	-2533.869725	0.00
8	-2533.878706	1.13
9	-2533.880345	6.39
10	-2533.878403	0.82
11	-2533.874358	0.01
12	-2533.880235	5.68
13	-2533.875925	0.06
14	-2533.881514	22.02
15	-2533.872851	0.00
16	-2533.879989	4.38
17	-2533.875945	0.06
18	-2533.873852	0.01
19	-2533.870127	0.00
20	-2533.877628	0.36
21	-2533.874522	0.01
22	-2533.875111	0.03
23	-2533.878019	0.54
24	-2533.878509	0.91
25	-2533.877011	0.19
26	-2533.871048	0.00

trans c(DSTAIPF)

1	-2533.852654	0.01
2	-2533.851802	0.00
3	-2533.852059	0.01
4	-2533.848038	0.00
5	-2533.853543	0.02
6	-2533.860919	61.40
7	-2533.858070	3.01
8	-2533.857292	1.32
9	-2533.852679	0.01
10	-2533.851022	0.00
11	-2533.859916	21.23
12	-2533.859233	10.30
13	-2533.847574	0.00
14	-2533.855595	0.22
15	-2533.853738	0.03
16	-2533.851562	0.00
17	-2533.849711	0.00
18	-2533.854626	0.08
19	-2533.848522	0.00
20	-2533.853891	0.04
21	-2533.857597	1.82
22	-2533.846874	0.00
23	-2533.856273	0.45
24	-2533.850127	0.00
25	-2533.850716	0.00
26	-2533.853869	0.04

Table S6. Geometry optimization at M06-2X/6-31G(d,p)/SMD level of theory for the 67 most important conformations for all studied cyclopeptides (conformation number, Energy in hartree and % population according to the Boltzmann distribution)

cis c(NSLAIPF)

1	-2518.707413	18.03
3	-2518.707876	29.45
6	-2518.705492	2.36
12	-2518.707876	29.45
20	-2518.705614	2.68
25	-2518.707413	18.03

trans c(NSLAIPF)

2	-2518.697327	36.04
17	-2518.696730	19.16
20	-2518.697327	36.05
21	-2518.695989	8.75

cis c(NSTAIPF)

1	-2515.315367	7.26
4	-2515.316544	25.23
6	-2515.315339	7.05
7	-2515.315842	11.99
8	-2515.314906	4.45
10	-2515.312922	0.54
22	-2515.316239	18.26
24	-2515.316544	25.22

trans c(NSTAIPF)

2	-2515.305469	0.83
14	-2515.306501	2.48
16	-2515.307924	11.16
17	-2515.304760	0.39
19	-2515.309599	65.76
22	-2515.303783	0.14
25	-2515.304761	0.39
26	-2515.308418	18.85

cis c(KSTAIPF)

1	-2520.344524	6.92
3	-2520.343963	3.82
5	-2520.343963	3.82
9	-2520.346686	68.28
21	-2520.344666	8.04
23	-2520.343120	1.57
24	-2520.343939	3.73
25	-2520.343963	3.82

trans c(KSTAIPF)

1	-2520.336164	0.38
2	-2520.334332	0.05
3	-2520.339586	14.22
4	-2520.340738	48.19
13	-2520.334499	0.07
16	-2520.340350	31.93
22	-2520.334420	0.06
23	-2520.338606	5.04
24	-2520.334269	0.05

cis c(RSTAIPF)

1	-2629.845126	7.71
5	-2629.845046	7.08
6	-2629.846435	30.80
8	-2629.843071	0.87
9	-2629.846739	42.51
10	-2629.845350	9.77
16	-2629.842285	0.38
19	-2629.843074	0.88

trans c(RSTAIPF)

2	-2629.834614	1.15
3	-2629.838511	71.12
4	-2629.837022	14.70
24	-2629.836908	13.03

cis c(DSTAIPF)

1	-2534.714724	5.40
5	-2534.715536	12.76
9	-2534.716937	56.20
12	-2534.715535	12.75
14	-2534.714876	6.34
16	-2534.714906	6.55

trans c(DSTAIPF)

6	-2534.692169	0.87
8	-2534.692355	1.06
11	-2534.692176	0.88
12	-2534.696403	77.21
21	-2534.695099	19.42
23	-2534.691738	0.55

Table S7. Single point calculations (geometries from M06-2X/6-31G(d)/SMD) at M06-2X/def2-TZVP/SMD level of theory for the 57 most important conformations for all studied cyclopeptides (conformation number, Energy in hartree and % population according to the Boltzmann distribution).

cis c(NSLAIPF)

1	-2519.629396	17.57
3	-2519.629947	31.49
6	-2519.627847	3.41
12	-2519.629507	19.75
20	-2519.627396	2.11
25	-2519.629754	25.67

trans c(NSLAIPF)

2	-2519.622017	40.71
17	-2519.620963	13.34
20	-2519.621974	38.90
21	-2519.62036	7.05

cis c(NSTAIPF)

1	-2516.249371	2.03
4	-2516.252222	41.61
6	-2516.250674	8.08
7	-2516.249083	1.50
8	-2516.249055	1.46
10	-2516.245240	0.03
22	-2516.249935	3.69
24	-2516.252222	41.60

trans c(NSTAIPF)

2	-2516.238981	0.09
14	-2516.242679	4.48
16	-2516.243737	13.73
17	-2516.240774	0.60
19	-2516.245191	64.01
22	-2516.240030	0.27
25	-2516.240817	0.62
26	-2516.243893	16.19

cis c(KSTAIPF)

1	-2521.261520	2.27
3	-2521.261354	1.90
5	-2521.261236	1.68
9	-2521.264396	47.64
21	-2521.264234	40.13
23	-2521.261469	2.15
24	-2521.261554	2.35
25	-2521.261345	1.88

trans c(KSTAIPF)

1	-2521.254321	1.07
2	-2521.252084	0.10
3	-2521.256384	9.49
4	-2521.258268	69.74
13	-2521.253924	0.70
16	-2521.257012	18.45
22	-2521.253037	0.27
23	-2521.252552	0.16
24	-2521.249549	0.01

cis c(RSTAIPF)

1	-2630.807463	16.31
5	-2630.806875	8.75
6	-2630.808040	30.05
8	-2630.804675	0.85
9	-2630.807673	20.37
10	-2630.807762	22.39
16	-2630.803314	0.20
19	-2630.804896	1.08

trans c(RSTAIPF)

2	-2630.798459	4.71
3	-2630.800624	46.57
4	-2630.800626	46.67
24	-2630.797676	2.06

cis c(DSTAIPF)

1	-2535.669458	5.18
5	-2535.669578	5.88
9	-2535.669310	4.43
12	-2535.669514	5.50
14	-2535.669060	3.40
16	-2535.671990	75.60

trans c(DSTAIPF)

6	-2535.653083	1.24
8	-2535.654141	3.79
11	-2535.650502	0.08
12	-2535.656724	58.36
21	-2535.656257	35.61
23	-2535.652807	0.92

Table S8. Single point calculations (geometries from M06-2X/6-31G(d)/SMD) at MP2/6-31G(d)/SMD level of theory for the 57 most important conformations for all studied cyclopeptides (conformation number, Energy in hartree and % population according to the Boltzmann distribution).

cis c(NSLAIPF)

1	-2504.316841	1.17
3	-2504.316617	0.93
6	-2504.319359	16.86
12	-2504.316466	0.79
20	-2504.320803	77.82
25	-2504.317531	2.43

trans c(NSLAIPF)

2	-2504.312607	12.56
17	-2504.314382	82.18
20	-2504.311749	5.06
21	-2504.308732	0.21

cis c(NSTAIPF)

1	-2501.114180	29.30
4	-2501.111947	2.75
6	-2501.108017	0.04
7	-2501.113022	8.60
8	-2501.114521	42.01
10	-2501.113500	14.26
22	-2501.109808	0.29
24	-2501.111946	2.75

trans c(NSTAIPF)

2	-2501.102831	0.49
14	-2501.106665	28.62
16	-2501.104513	2.94
17	-2501.106746	31.20
19	-2501.106477	23.46
22	-2501.104933	4.57
25	-2501.105541	8.71

cis c(KSTAIPF)

1	-2505.914361	0.35
3	-2505.917399	8.70
5	-2505.917100	6.34
9	-2505.911817	0.02
21	-2505.913534	0.15
23	-2505.918709	34.84
24	-2505.918651	32.75
25	-2505.918024	16.85

trans c(KSTAIPF)

1	-2505.910100	0.56
2	-2505.911476	2.42
3	-2505.911754	3.25
4	-2505.910507	0.87
13	-2505.914916	92.53
16	-2505.909099	0.20
22	-2505.908848	0.15
23	-2505.906388	0.01
24	-2505.899641	0.00

cis c(RSTAIPF)

1	-2614.845018	9.17
5	-2614.841877	0.33
6	-2614.841893	0.34
8	-2614.834032	0.00
9	-2614.842518	0.65
10	-2614.846707	54.81
16	-2614.846276	34.71
19	-2614.836786	0.00

trans c(RSTAIPF)

2	-2614.840864	90.40
3	-2614.835869	0.46
4	-2614.838699	9.14
24	-2614.819350	0.00

cis c(DSTAIPF)

1	-2520.477381	73.67
5	-2520.472994	0.71
9	-2520.474826	4.92
12	-2520.472255	0.32
14	-2520.475644	11.71
16	-2520.475360	8.67

trans c(DSTAIPF)

6	-2520.458103	0.15
8	-2520.463863	66.06
11	-2520.461431	5.03
12	-2520.462649	18.27
21	-2520.460691	2.30
23	-2520.461891	8.19

Table S9. Average intramonomeric and intermonomeric relevant distances (Å) of the *trans,trans* dimeric cyclopeptides.[a]

Type	*Residues*	*Mono-mer*	*c(NSLAIPF)*	*c(NSTAIPF)*	*c(KSTAIPF)*	*c(RSTAIPF)*	*c(DSTAIPF)*
Type II β-turn	S^2_i-T^3_{i+1}-A^4_{i+2}-I^5_{i+3} [a]	A	3.8±0.3	3.7±0.3	3.7±0.3	3.8±0.3	3.7±0.3
		B	3.6±0.3	3.8±0.3	3.7±0.3	3.8±0.3	3.6±0.3
γ-turn	F^7_i-K^1_{i+1}-S^2_{i+2} [a]	A	2.9±0.1	2.8±0.1	2.8±0.1	2.8±0.1	2.8±0.1
		B	2.8±0.2	2.8±0.1	2.8±0.1	2.8±0.1	2.8±0.1
γ-turn	I^5_i-P^6_{i+1}-F^7_{i+2} [a]	A	3.1±0.2	3.0±0.2	3.0±0.2	3.0±0.2	3.0±0.2
		B	3.0±0.2	3.0±0.2	3.0±0.2	3.1±0.2	3.0±0.2
Intermonomeric hydrogen bond 1	A^4 (A) – S^2 (B) [b]	-	3.0±0.3	3.0±0.2	3.0±0.2	3.3±0.7	3.0±0.2
Intermonomeric hydrogen bond 2	S^2 (A) – A^4 (B) [b]	-	3.0±0.4	3.0±0.2	3.0±0.2	3.3±0.7	3.0±0.2
Pro-Pro distance	P^6 (A) – P^6 (B) [c]	-	4.4±0.4	4.3±0.3	4.3±0.3	4.6±0.6	4.3±0.3

[a] Distance from carbonyl oxygen of residue i and the nitrogen of the NH unit of residue i+2 (γ-turn) and i+3 (β-turn)

[b] Distance from carbonyl oxygen of the first residue in monomer A and the nitrogen of the peptide unit of the second residue in monomer B.

[c] Distance from the nitrogen of the NH unit of Pro residue in monomer A and the analogous of monomer B.

Table S10. Phi and psi backbone torsional angles (degrees) and distances (Å) of β- and γ-turns in the dimeric species of *trans,trans* c(KSTAIPF).[a]

Monomer	ϕ_{i+1}	Ψ_{i+1}	ϕ_{i+2}	Ψ_{i+2}	d_1[a]	d_2[b]
Type II β-turn: S^2_i-T^3_{i+1}-A^4_{i+2}-I^5_{i+3}						
A	-67±11	135±9	59±8	22±10	5.8±0.4	3.7±0.3
B	-67±11	136±9	59±8	23±10	5.8±0.4	3.7±0.3
γ-turn: F^7_i-K^1_{i+1}-S^2_{i+2}						
A	55±14	-34±28			5.9±0.1	2.8±0.1
B	55±9	-35±27			5.9±0.1	2.8±0.1
γ-turn: I^5_i-P^6_{i+1}-F^7_{i+2}						
A	-65±9	-4±15			5.6±0.2	3.0±0.2
B	-65±9	-3±15			5.6±0.2	3.0±0.2

[a] Distance between C_α carbons of residues i and i+2 (γ-turn) or i+3 (β-turn).

[b] Distance from carbonyl oxygen of residue i and the nitrogen of the peptide unit of residue i+2 (γ-turn) and i+3 (β-turn). See Table S4 for the values of other cyclopeptides.

Figure S1. General method used for cyclopeptide preparation.

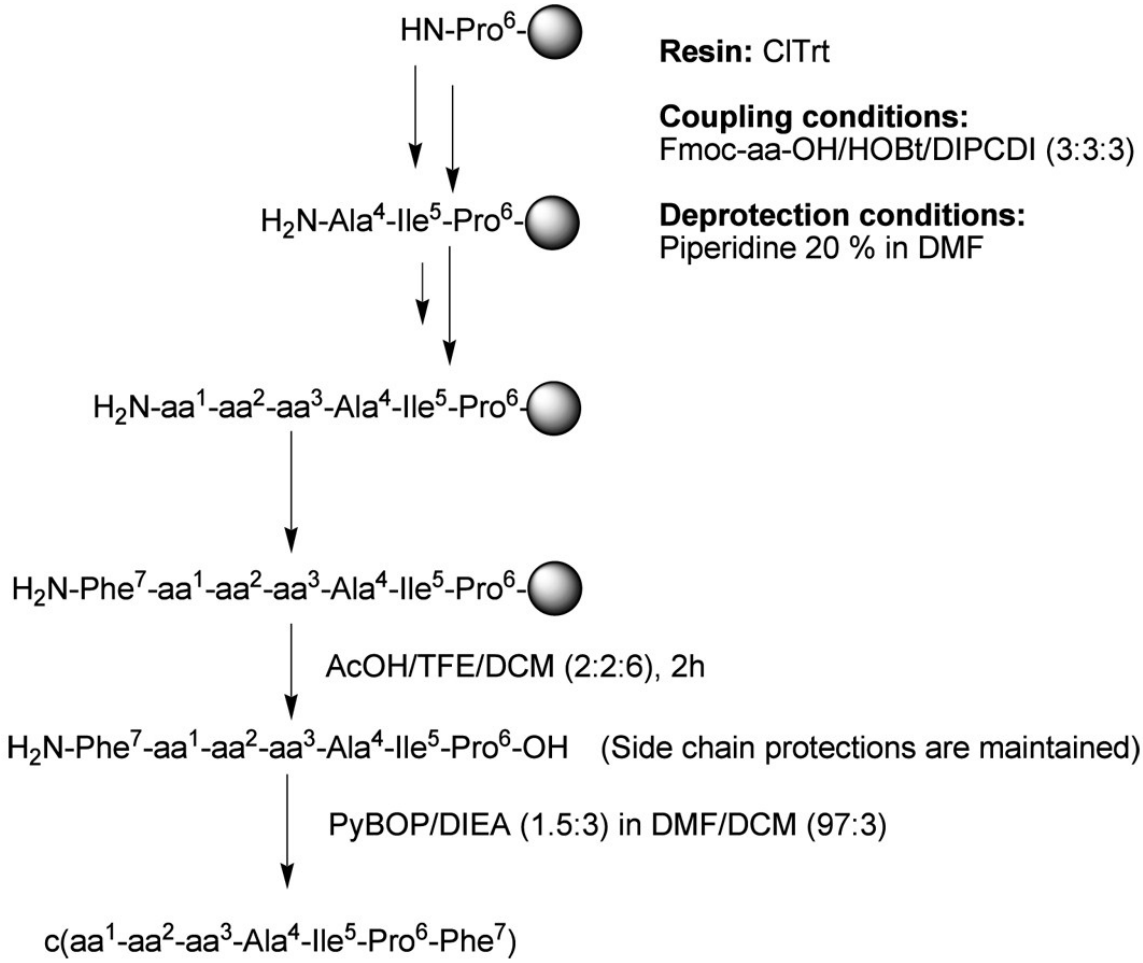


Figure S2. Circular dichroism spectra of all studied cyclopeptides (c(NSLAIPF), c(NSTAIPF), c(KSTAIPF), c(RSTAIPF) and c(DSTAIPF) recorded at increasing cyclopeptide concentration.

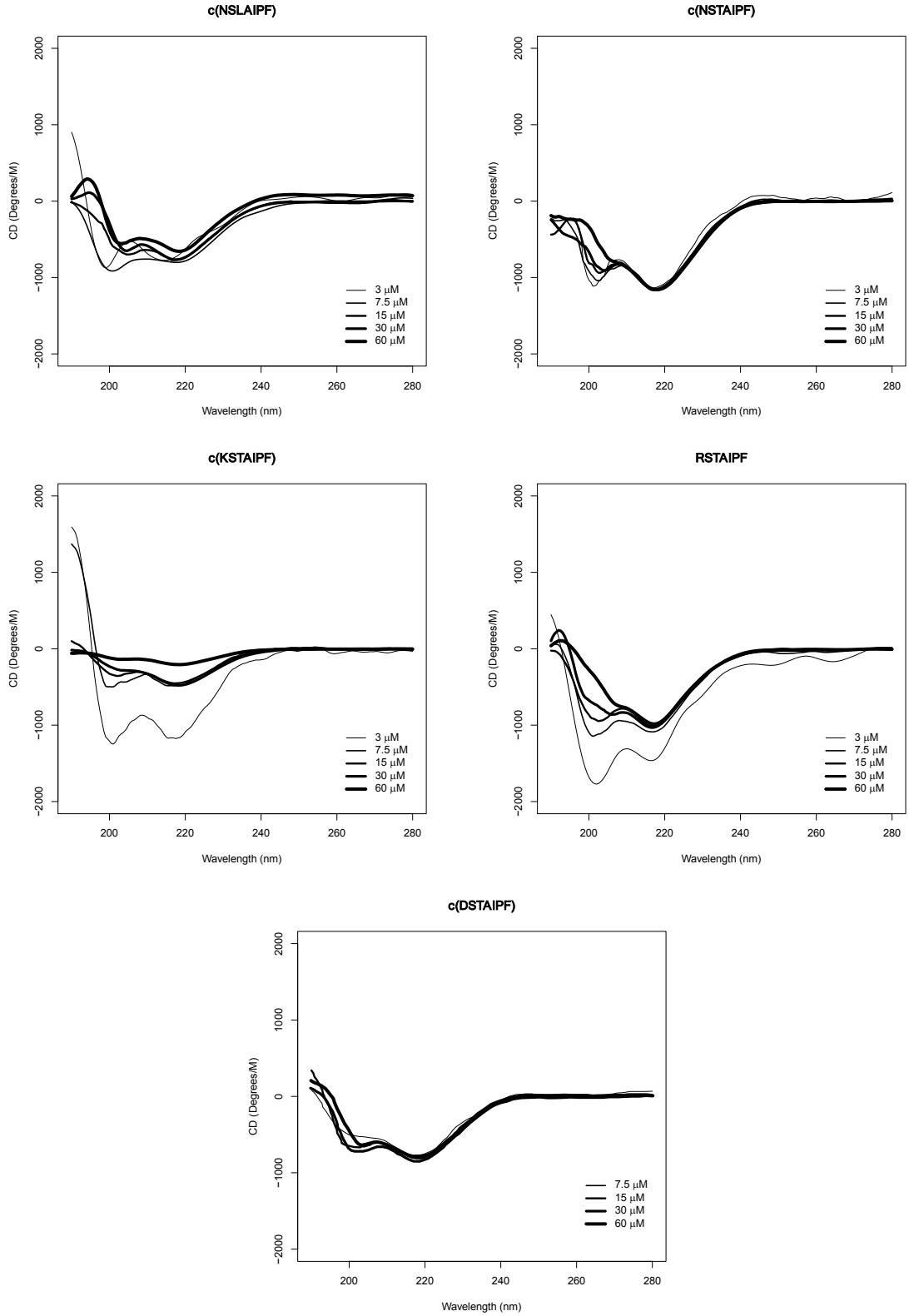
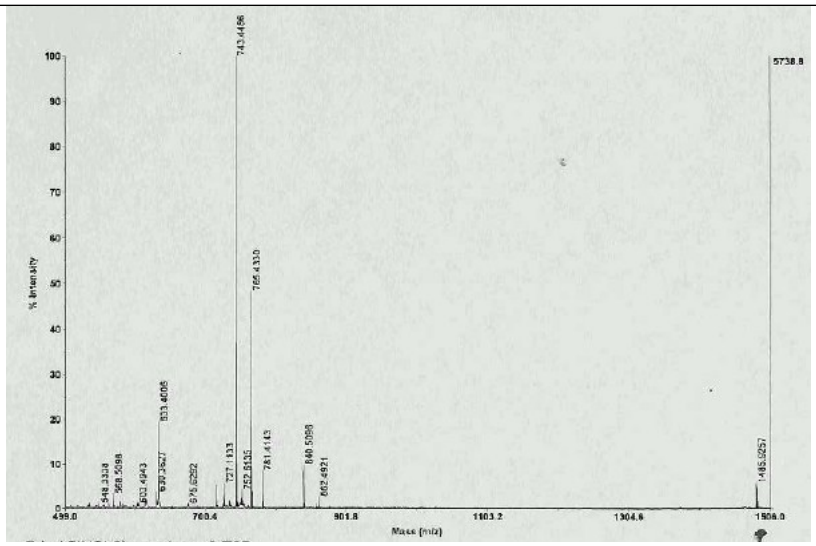
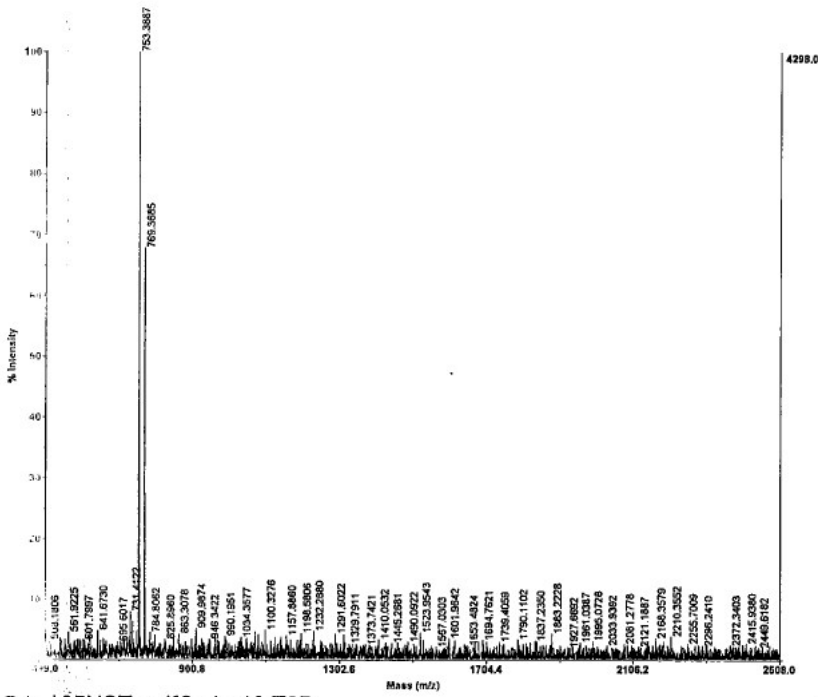


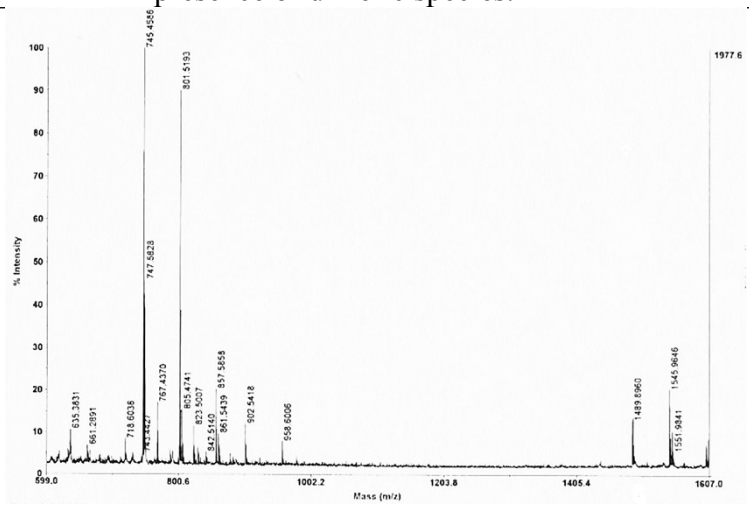
Figure S3. MALDI-TOF spectra recorded for c(NSLAIPF), c(NSTAIPF), c(KSTAIPF), c(RSTAIPF) and c(DSTAIPF).



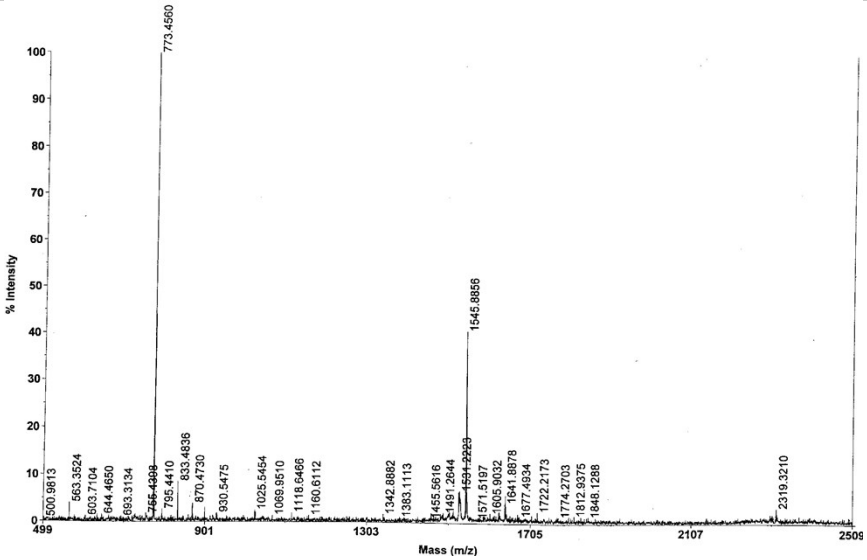
c(NSLAIPF). The peak at 743.4496 m/z and 1485.6267 m/z correspond to monomer and dimer species respectively.



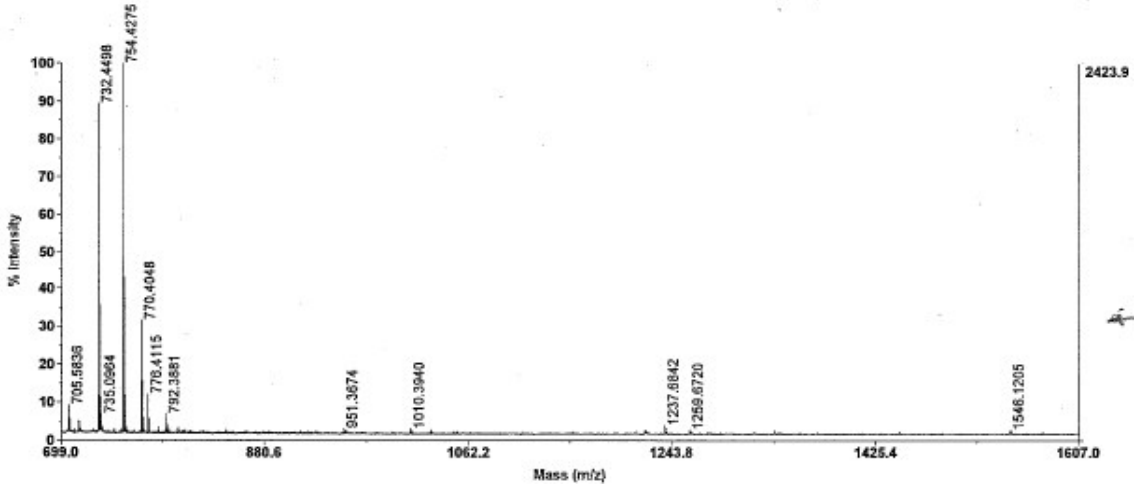
c(NSTAIPF). The peak at 753.3887 m/z correspond to monomer with the addition of Na atom. There is no presence of dimeric species.



c(KSTAIPF). The peak at 745.4586 m/z and 1489.8960 m/z correspond to monomer and dimeric species, respectively.

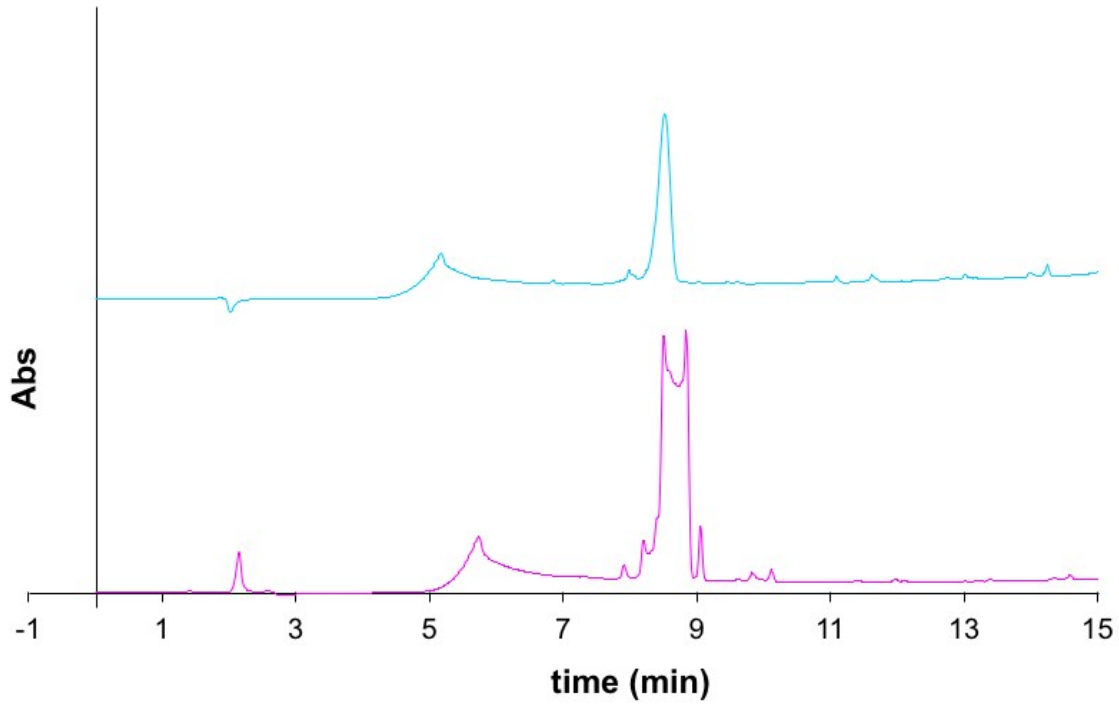


c(RSTAIPF). The peak at 773.4560 m/z and 1545.8856 m/z correspond to monomer and dimeric species, respectively.



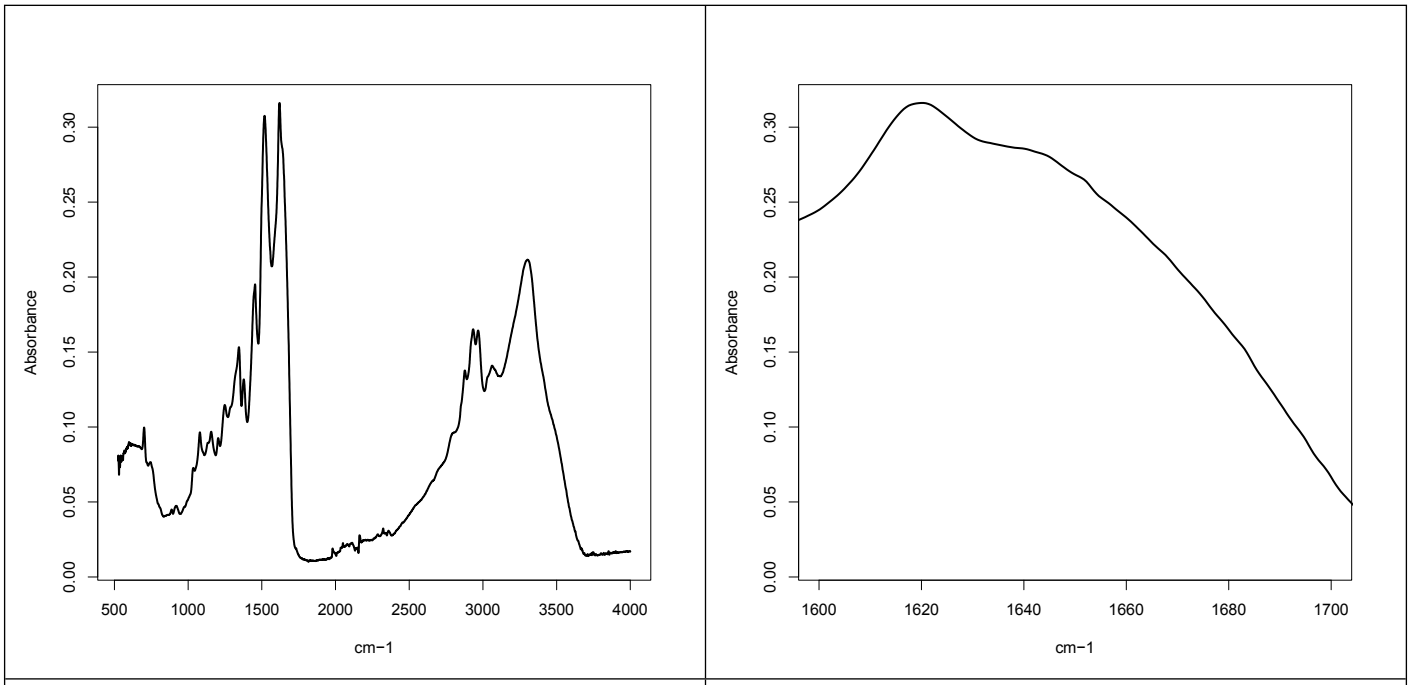
c(DSTAIPF). The peak at 732.4498 m/z correspond to the monomer and 754.4265 m/z correspond to monomer with the addition of Na atom. There is no presence of dimeric species.

Figure S4. HPLC chromatogram of c(KSTAIPF) at room temperature (magenta) and 45°C (cyan).



Upon temperature increase from room temperature to 45°C the most relevant peaks coalesce into a single peak. This might be explained by the existence of different species of c(KSTAIPF) in water. This could be interpreted as the existence of different conformational states, such as an equilibrium between the monomeric *cis* and *trans* species and the dimeric form, when one considers these data in light of the experimental and theoretical results reported in this work. Nevertheless, the chromatogram also reveals the existence of other minor peaks, near the main peak, which could reflect the existence of a lowly populated conformations; and also far away from it, which could perhaps be attributed to impurities generated during the synthesis of the cyclic peptide.

Figure S5. IR spectrum of a solid sample of c(KSTAIPF) registered using a Thermo Scientific Nicolet iZ10 FTIR system.



(a) 525-4000 cm^{-1} range | (b) 1600-1700 cm^{-1} range

The spectrum was recorded in the 525–4000 cm^{-1} range with 32 scans at a resolution of 4 cm^{-1}. The IR spectrum is an averaged spectrum of the cis and trans conformations since the synthesis of c(KSTAIPF) yields a mixture of the two. However, the overall shape of the amide-I band of both conformations should be very similar as both contain intramolecular hydrogen bonds formed of peptide carbonyl groups and also peptide carbonyl extending out into the solvent; see Figure 5

Figure S6. ROESY experiments showing in circles the exchange of signals for specific residues in the *trans* (_t; green) and *cis* (_c; purple) conformers.

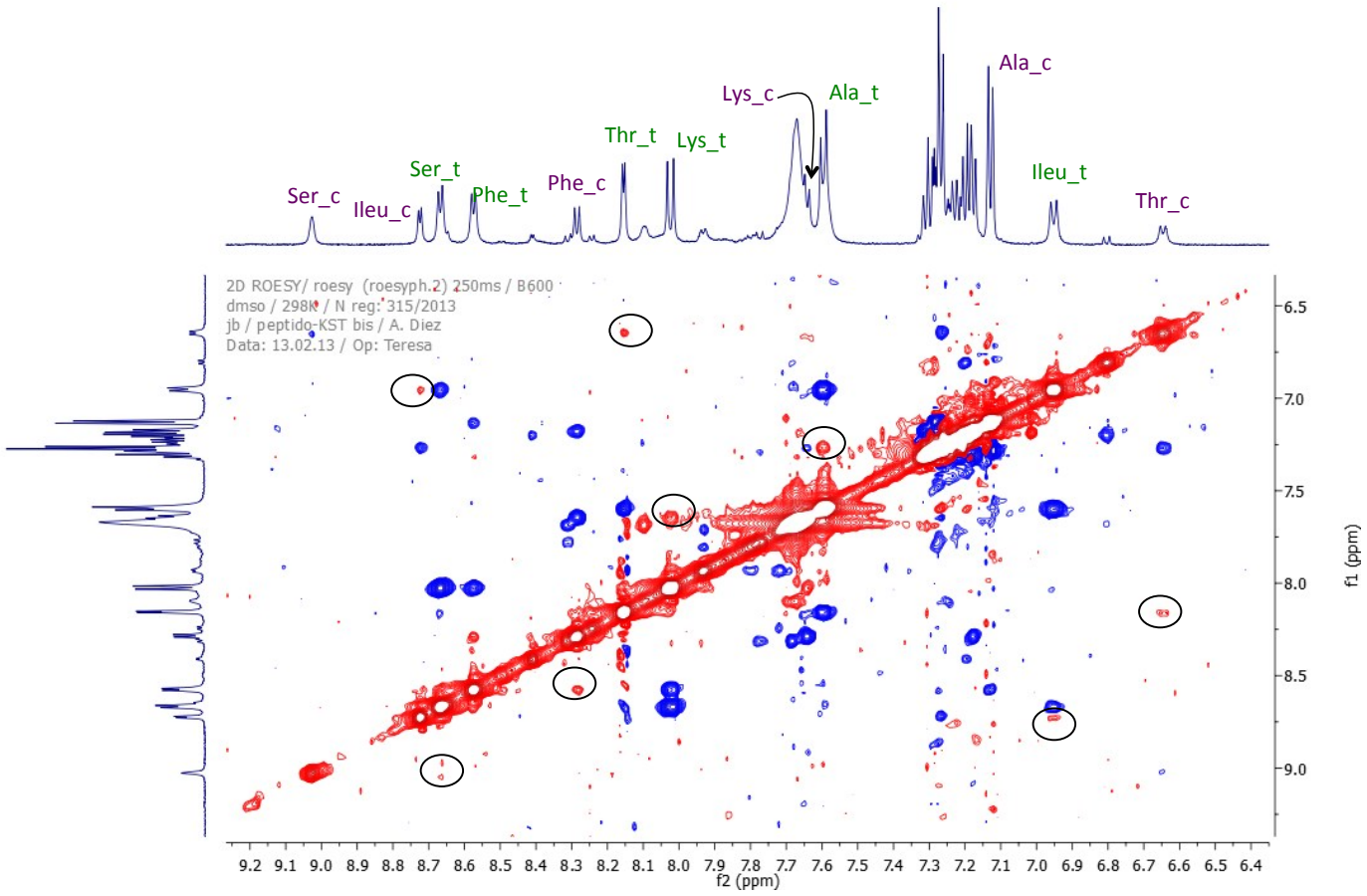
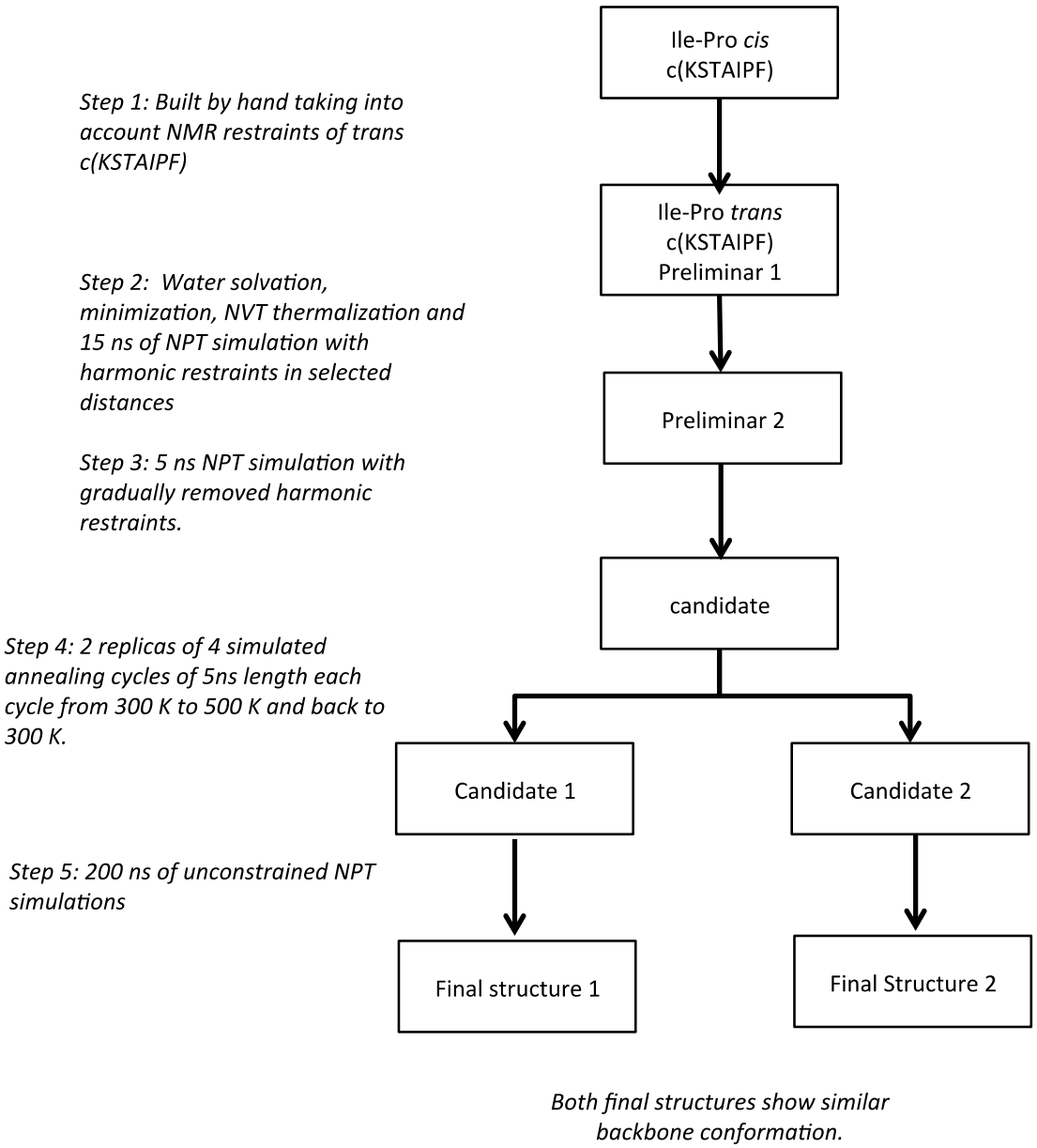
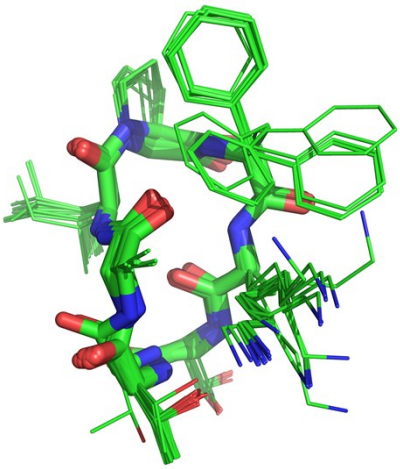


Figure S7. Computational protocol for structural elucidation of the *trans* monomeric form of c(KSTAIPF; see Experimental section for more details).

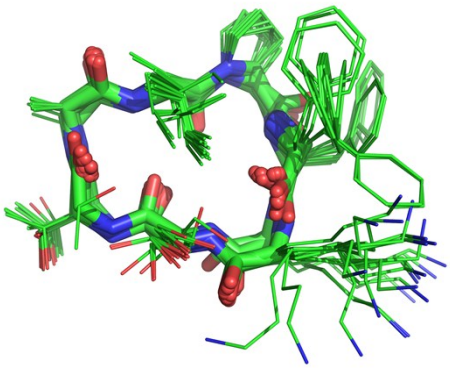


Both final structures show similar backbone conformation.

Figure S8. Conformational ensemble optimized at the M06-2X/6-31G(d)/SMD level of computation for *cis* and *trans* conformers of c(KSTAIPF) used to determine the relative Gibbs free energies between both conformers. Here 25 and 24 conformations of (left) *cis* and (right) *trans* c(KSTAIPF), respectively, are represented. This is an illustrative example of the conformational space explored by the 256 conformations of the five *cis* and *trans* conformers of cyclopeptides, see Table S3. Backbone as bold sticks, side chain as thin sticks. Hydrogens are omitted. Green, red and blue for carbon, oxygen and nitrogen atoms, respectively.



cis c(KSTAIPF)



trans c(KSTAIPF)

Figure S9. Computational protocol for structural elucidation of the *trans,trans* dimeric form of c(KSTAIPF; see Experimental section for more details). The name of the five relative orientations denotes the residues of both peptides that are placed facing each other in the initial structure. Identical protocols were applied to the *cis,cis* and *cis,trans* dimeric forms, but in this latter case after step 4 all MD simulations led to an unbound structure.

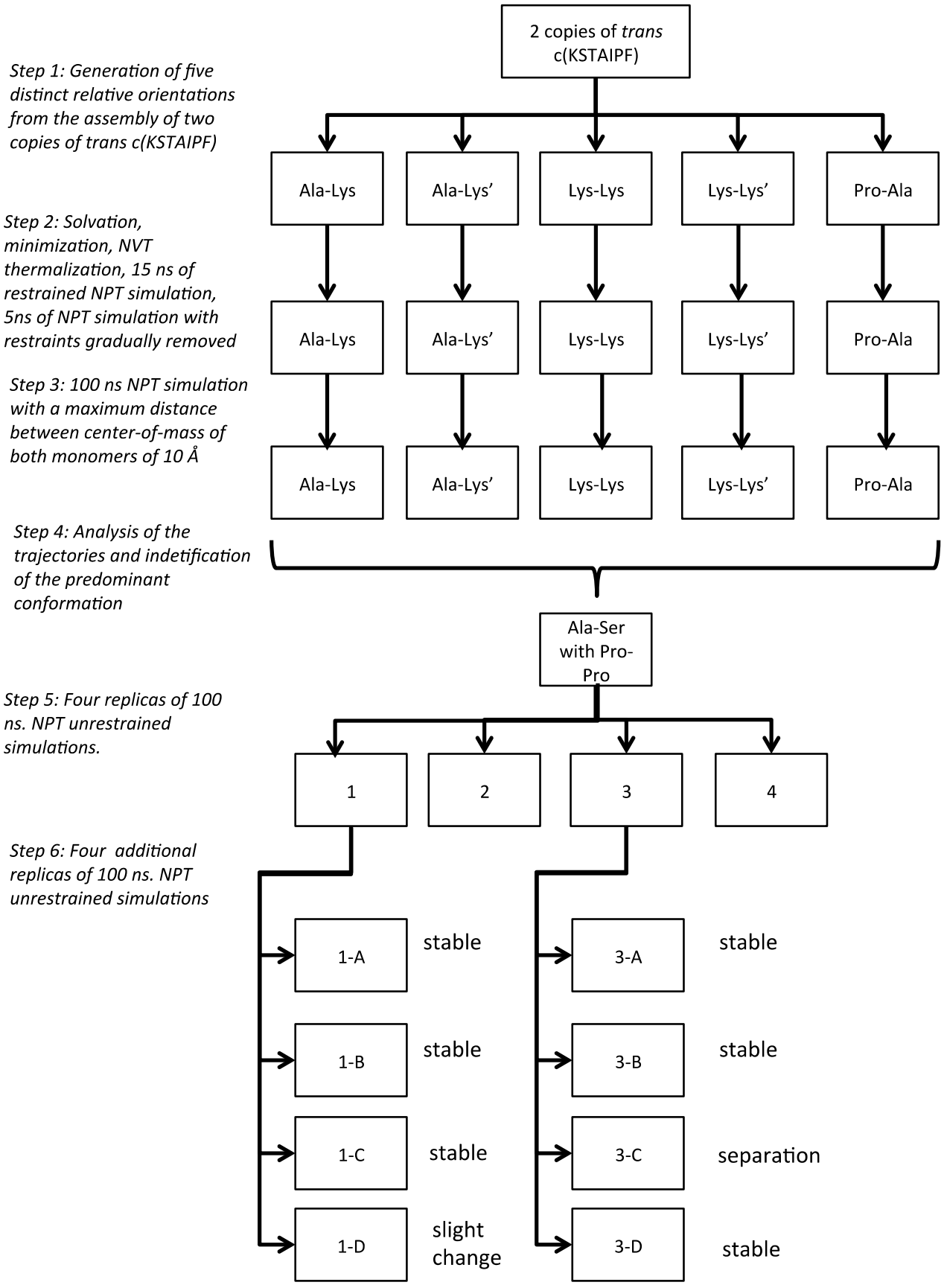
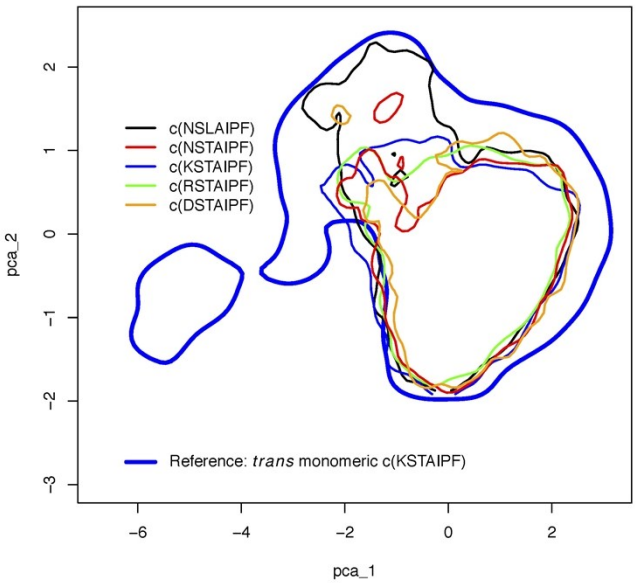
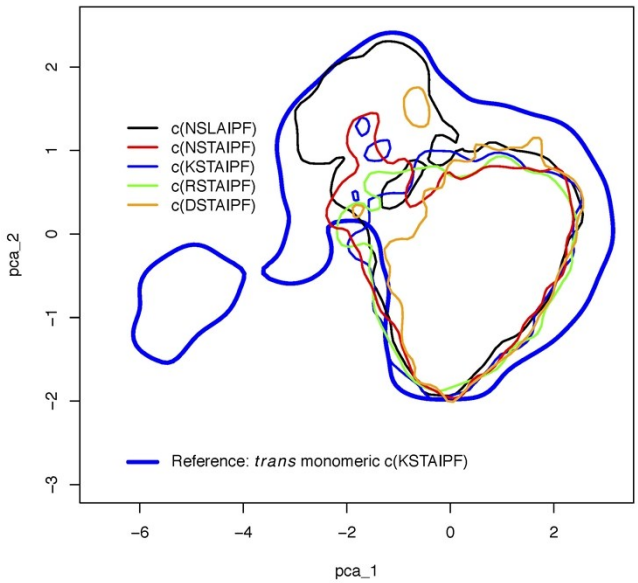


Figure S10. Conformational analysis of both monomers (A and B) of the *trans,trans* dimeric cyclopeptides. The plot shows the contour map (isodensity lines) of the projection of the backbone cartesian coordinates of MD simulations of both monomers (a and b, respectively) of all *trans,trans* dimer cyclopeptides over the same conformational space of *trans* monomeric c(KSTAIPF) taken as a reference by principal component analysis. The same procedure as explained in Figure 6 is applied here.



(a) Monomer A. Residues 1-7



(b) Monomer B. Residues 8-14

Figure S11. Optimized Cartesian coordinates (M06-2X/6-31G(d)/SMD) of the most populated conformations (conformation number and % of population according to the Boltzmann distribution) of *cis* and *trans* monomeric cyclopeptides and the most representative structure of the MD simulations of the *trans,trans* dimeric c(KSTAIPF) in PDB format.

***cis* c(NSLAIPF), conformation 20, 35 %**

N	1.80069	1.33740	3.31192
C	1.58473	1.83731	4.68380
H	0.52943	2.08363	4.83545
H	2.17143	2.75039	4.82393
C	2.06584	0.68949	5.57767
H	1.21981	0.05760	5.86742
H	2.54146	1.05702	6.48830
C	3.02706	-0.09691	4.68109
H	3.99572	0.40617	4.61324
H	3.18492	-1.12836	4.99936
C	2.33528	-0.02394	3.31192
H	3.03377	-0.19364	2.48919
C	1.25181	-1.10689	3.24397
O	1.56043	-2.29779	3.34184
N	-0.02333	-0.70152	3.12737
H	-0.22419	0.26770	2.90118
C	-1.11205	-1.65816	3.10972
H	-1.05214	-2.28394	4.00620
C	-2.46001	-0.91662	3.08225
H	-3.25001	-1.67396	3.10740
H	-2.54078	-0.37085	2.13627
C	-2.59321	0.03744	4.24432
C	-2.95454	-0.43410	5.50983
H	-3.18100	-1.48996	5.64043
C	-3.02835	0.43399	6.59612
H	-3.31565	0.05424	7.57207
C	-2.73736	1.78820	6.43131
H	-2.79529	2.46543	7.27790
C	-2.37420	2.26769	5.17465
H	-2.14622	3.32058	5.03599
C	-2.30230	1.39646	4.08777
H	-2.01244	1.77478	3.10816
C	-1.02707	-2.61275	1.91759
O	-1.39668	-3.78566	2.01128
N	-0.57637	-2.06557	0.77908
H	-0.28100	-1.08957	0.76763
C	-0.36336	-2.84121	-0.42206
H	0.07969	-3.80528	-0.14456
C	-1.68190	-3.13393	-1.15792
H	-1.49527	-3.70533	-2.07213
H	-2.30438	-3.74342	-0.49908
C	-2.37981	-1.85026	-1.54007
O	-1.86968	-1.07458	-2.36697
N	-3.54573	-1.60015	-0.94494
H	-3.92533	-2.22939	-0.24929
H	-4.04924	-0.74722	-1.16153
C	0.67296	-2.08515	-1.25466
O	1.17733	-1.03972	-0.84013
N	1.03774	-2.62910	-2.42741
H	0.59695	-3.47721	-2.76809
C	2.11096	-2.03511	-3.20173
H	3.01623	-1.96824	-2.58910
C	2.41395	-2.89961	-4.41550
H	2.70559	-3.90260	-4.08211
H	3.25380	-2.44893	-4.95600
O	1.24193	-2.94509	-5.21412
H	1.42018	-3.52882	-5.96784
C	1.81717	-0.61147	-3.67932
O	2.75993	0.10128	-4.04107
N	0.53072	-0.24800	-3.74584
H	-0.19093	-0.87648	-3.39355
C	0.10817	1.03987	-4.27461
H	0.94959	1.44920	-4.83612
C	-1.10938	0.87694	-5.18903
H	-1.29981	1.84832	-5.66351
H	-1.99733	0.63019	-4.59388
C	-0.92038	-0.20250	-6.26281
H	-0.89653	-1.17708	-5.75714
C	-2.11316	-0.18771	-7.21700
H	-2.15269	0.75919	-7.76893
H	-2.04193	-0.99971	-7.94802
H	-3.05861	-0.30024	-6.67534
C	0.38997	-0.03787	-7.03148
H	0.44132	0.95247	-7.50143
H	1.26728	-0.15065	-6.38440
H	0.46568	-0.78945	-7.82458
C	-0.11846	2.00550	-3.10723
O	0.64187	2.96210	-2.91117
N	-1.16546	1.72388	-2.31019
H	-1.64120	0.82532	-2.41852
C	-1.38286	2.41372	-1.04230
H	-1.08915	3.45758	-1.18151
C	-2.83676	2.31876	-0.62314
H	-3.47611	2.79016	-1.37261
H	-3.13505	1.27310	-0.50629
H	-2.98446	2.82398	0.33478
C	-0.46179	1.78906	0.01083
O	-0.87644	0.99308	0.86641
N	0.82618	2.13620	-0.07642
H	1.10762	2.76938	-0.82012
C	1.80079	1.60336	0.85385
H	1.71928	0.51170	0.83466
C	3.23310	1.99360	0.42951
H	3.90331	1.51043	1.15385
C	3.53779	1.41799	-0.95728
H	2.96789	1.93176	-1.74171
H	4.59973	1.52576	-1.19383
H	3.28946	0.35278	-0.99922
C	3.48303	3.50674	0.50347
H	3.28215	3.85559	1.52243
H	2.77937	4.03609	-0.15355
C	4.90956	3.89057	0.11710
H	5.10307	3.71584	-0.94516
H	5.09071	4.95080	0.31655
H	5.63984	3.31026	0.69272
C	1.46614	2.11389	2.26135
O	0.93696	3.21672	2.43347

trans c(NSLAIPF), conformation 21, 30 %

N	1.20883	2.97172	1.75721
C	1.37220	4.43350	1.74441
H	0.41034	4.90100	1.50762
H	2.10743	4.74946	1.00700
C	1.78217	4.72568	3.18284
H	1.63428	5.77355	3.45078
H	2.83756	4.47079	3.31966
C	0.87846	3.78125	3.97780
H	1.27938	3.52022	4.95836
H	-0.10335	4.23802	4.12148
C	0.72581	2.53630	3.08571
H	1.35784	1.70601	3.41931
C	-0.72597	2.02257	3.06934
O	-1.56996	2.44225	3.85860
N	-0.98447	1.04415	2.17176
H	-0.24156	0.77924	1.52412
C	-2.33188	0.57619	1.90894
H	-2.92037	0.75653	2.81641
C	-2.98518	1.31728	0.72921
H	-3.95600	0.85470	0.53478
H	-2.35919	1.17615	-0.16168
C	-3.16123	2.78137	1.04051
C	-4.31615	3.21961	1.69574
H	-5.09802	2.50056	1.92999
C	-4.47338	4.55772	2.04696
H	-5.37768	4.88083	2.55416
C	-3.47422	5.48118	1.74282
H	-3.59748	6.52683	2.00774
C	-2.31857	5.05563	1.09096
H	-1.54218	5.77306	0.84032
C	-2.16020	3.71261	0.74912
H	-1.24931	3.38108	0.25419
C	-2.34095	-0.92963	1.66693
O	-3.17284	-1.45407	0.91505
N	-1.41916	-1.66046	2.31472
H	-0.70860	-1.18312	2.85827

C	-1.24985	-3.07597	2.01677
H	-0.28937	-3.37572	2.44402
C	-2.34381	-3.95311	2.61153
H	-3.31078	-3.73878	2.15147
H	-2.41962	-3.74202	3.68365
C	-1.98736	-5.41823	2.46186
O	-0.81328	-5.80279	2.46543
N	-3.02425	-6.26367	2.36985
H	-2.84856	-7.25890	2.31454
H	-3.97915	-5.93238	2.36263
C	-1.15959	-3.28881	0.49447
O	-1.76041	-4.20199	-0.06902
N	-0.34003	-2.42771	-0.13622
H	0.08034	-1.66688	0.39116
C	-0.26771	-2.29212	-1.57667
H	-0.50076	-3.25701	-2.03376
C	-1.27190	-1.23401	-2.06080
H	-1.13401	-1.06001	-3.13270
H	-1.06044	-0.29998	-1.52354
O	-2.60594	-1.64865	-1.85977
H	-2.81681	-1.53767	-0.91273
C	1.14764	-1.85307	-1.92653
O	1.80227	-1.15839	-1.14048
N	1.61950	-2.22841	-3.12166
H	1.06191	-2.84205	-3.70712
C	3.00770	-1.99840	-3.49291
H	3.64520	-2.63610	-2.87062
C	3.18914	-2.33746	-4.97430
H	2.49434	-1.70914	-5.54503
H	2.88807	-3.38309	-5.12373
C	4.61256	-2.14333	-5.50767
H	4.89699	-1.09062	-5.36374
C	5.62716	-3.02773	-4.78304
H	5.72130	-2.77656	-3.72132
H	5.33306	-4.08210	-4.85505
H	6.61874	-2.92212	-5.23533
C	4.63013	-2.43758	-7.00659
H	5.62675	-2.26840	-7.42665
H	4.35996	-3.48399	-7.19328
H	3.91954	-1.80333	-7.54670
C	3.38652	-0.53484	-3.26660
O	2.75071	0.38141	-3.79284
N	4.47978	-0.34215	-2.50743
H	4.93485	-1.15716	-2.11417
C	5.15026	0.93880	-2.35680
H	5.99370	0.75256	-1.68481
C	5.69582	1.46774	-3.68361
H	6.25898	2.38657	-3.51405
H	6.36454	0.72276	-4.12210
H	4.88415	1.67577	-4.38485
C	4.31836	2.01165	-1.64952
O	4.74825	3.17002	-1.64022
N	3.19272	1.64040	-1.01214
H	2.84077	0.68858	-1.09906
C	2.33437	2.64249	-0.40508
H	2.98154	3.49282	-0.18323
C	1.19937	3.11683	-1.35029
H	0.65448	3.90479	-0.80912
C	1.77793	3.73638	-2.62155
H	0.98505	4.19844	-3.21609
H	2.51405	4.50940	-2.38329
H	2.26497	2.97414	-3.24129
C	0.21577	1.98144	-1.65760
H	-0.16812	1.57111	-0.71253
H	0.75138	1.16142	-2.15712
C	-0.96336	2.42202	-2.52213
H	-1.71765	1.63094	-2.59086
H	-1.44937	3.31071	-2.10207
H	-0.64786	2.66297	-3.54164
C	1.74120	2.09118	0.88896
O	1.68977	0.86737	1.09357

cis **c(NSTAIPF), conformation 1, 37 %**

N	0.59629	-1.39022	-4.01445
C	0.01550	-2.25678	-5.05828
H	-0.61658	-3.02371	-4.60163
H	0.82545	-2.75778	-5.59793
C	-0.75962	-1.28521	-5.94945
H	-1.79575	-1.20122	-5.60395
H	-0.77211	-1.61066	-6.99076
C	-0.02582	0.04344	-5.74659
H	0.91859	0.04911	-6.29838
H	-0.60769	0.92253	-6.02697
C	0.28274	0.02109	-4.24155
H	1.12003	0.67478	-3.98530
C	-0.94454	0.51758	-3.46980
O	-1.35578	1.66841	-3.63899
N	-1.55751	-0.35630	-2.65494
H	-1.11573	-1.24809	-2.45062
C	-2.75356	0.01183	-1.92668
H	-3.46040	0.48037	-2.61863
C	-3.39483	-1.24115	-1.29972
H	-4.33211	-0.92849	-0.82998
H	-2.72950	-1.61776	-0.51439
C	-3.63663	-2.31422	-2.33284
C	-2.72502	-3.36246	-2.49002
H	-1.86140	-3.42402	-1.82964
C	-2.90952	-4.32216	-3.48511
H	-2.19253	-5.13067	-3.59386
C	-4.00870	-4.24089	-4.33718
H	-4.15492	-4.98687	-5.11221
C	-4.92345	-3.19861	-4.18710
H	-5.78504	-3.13256	-4.84474
C	-4.73725	-2.24198	-3.19197
H	-5.45254	-1.43076	-3.07703
C	-2.49016	1.03037	-0.81880
O	-3.38762	1.77591	-0.41839
N	-1.25772	1.01002	-0.28372
H	-0.59899	0.27951	-0.55112
C	-0.93422	1.80933	0.87202
H	-1.35252	2.81163	0.73968
C	-1.50395	1.16792	2.16589
H	-2.53703	0.87592	1.95563
H	-0.92434	0.27779	2.43191
C	-1.48010	2.13032	3.33226
O	-0.62458	2.05888	4.23457
N	-2.40863	3.08631	3.31074
H	-3.09742	3.12823	2.56871
H	-2.42521	3.79063	4.03933
C	0.58059	1.87051	0.97262
O	1.27915	0.98105	0.47154
N	1.11666	2.86044	1.69622
H	0.52682	3.55053	2.15242
C	2.52954	2.82166	2.03523
H	3.13763	2.90593	1.12963
C	2.85083	3.98703	2.96034
H	2.69781	4.92680	2.41767
H	3.90459	3.92044	3.25531
O	1.98204	3.89680	4.07838
H	2.09258	4.70391	4.60436
C	2.93895	1.49587	2.68774
O	4.06007	1.02811	2.48355
N	2.03901	0.92087	3.50626
H	1.14240	1.38362	3.67274
C	2.32949	-0.30797	4.21645
H	3.37659	-0.30171	4.53587
C	1.42471	-0.43329	5.45648
H	1.69236	-1.37837	5.93715
C	1.62586	0.71402	6.43390
H	2.66403	0.74519	6.77708
H	1.38749	1.67779	5.97170
H	0.97437	0.57430	7.30059
O	0.06616	-0.56689	5.05797
H	-0.27165	0.32006	4.81560
C	2.13527	-1.56858	3.37111
O	2.45592	-2.66924	3.83062
N	1.58321	-1.40819	2.16026
H	1.30514	-0.47703	1.86344
C	1.16928	-2.54339	1.34263
H	1.98930	-3.26955	1.33971
C	-0.10346	-3.18689	1.87214
H	0.06424	-3.53480	2.89424
H	-0.92313	-2.46309	1.87160
H	-0.38766	-4.04166	1.25221
C	0.98030	-2.01473	-0.07972
O	-0.14378	-1.87290	-0.57971
N	2.09200	-1.68047	-0.74253
H	2.99348	-1.77793	-0.28835
C	1.99268	-0.99439	-2.01614
H	1.33669	-0.12618	-1.87285

C	3.37432	-0.48811	-2.48378
H	3.21877	-0.06870	-3.48716
C	3.85103	0.64339	-1.56916
H	3.12119	1.45916	-1.55170
H	3.99805	0.29760	-0.53813
H	4.80141	1.05195	-1.92311
C	4.40695	-1.61756	-2.61047
H	3.95210	-2.46851	-3.12890
H	4.69166	-1.97333	-1.61146
C	5.66360	-1.18656	-3.36276
H	6.20455	-0.39587	-2.83472
H	6.34879	-2.03051	-3.48489
H	5.40962	-0.81231	-4.36065
C	1.35021	-1.93937	-3.03972
O	1.52755	-3.16026	-2.98889

trans **c(NSTAIPF), conformation 15, 37 %**

N	-1.52948	-2.55556	1.86769
C	-2.92345	-2.86996	2.24547
H	-3.59889	-2.04770	1.99753
H	-2.97992	-3.06421	3.32146
C	-3.21798	-4.12988	1.42799
H	-3.55536	-3.85043	0.42326
H	-3.98994	-4.74550	1.89314
C	-1.85729	-4.82531	1.34669
H	-1.62165	-5.32450	2.29079
H	-1.78401	-5.55476	0.53750
C	-0.88379	-3.65285	1.15007
H	0.10930	-3.85324	1.55742
C	-0.69028	-3.34287	-0.33146
O	0.09473	-4.01828	-1.00942
N	-1.42559	-2.34687	-0.84583
H	-2.05712	-1.83783	-0.23530
C	-1.47853	-2.02383	-2.26270
H	-1.33699	-2.96013	-2.81709
C	-2.83512	-1.40290	-2.60463
H	-2.89156	-1.30372	-3.69280
H	-2.87484	-0.39313	-2.18361
C	-3.98644	-2.22267	-2.07403
C	-4.80539	-1.72067	-1.05886
H	-4.62553	-0.71712	-0.67738
C	-5.84949	-2.48723	-0.53949
H	-6.47840	-2.07985	0.24679
C	-6.08175	-3.77038	-1.02847
H	-6.89230	-4.37019	-0.62571
C	-5.26687	-4.28166	-2.03971
H	-5.44344	-5.28064	-2.42736
C	-4.22829	-3.51297	-2.55787
H	-3.59671	-3.91520	-3.34712
C	-0.32994	-1.08502	-2.66460
O	-0.51572	-0.04344	-3.29470
N	0.89953	-1.49458	-2.28592
H	0.99155	-2.42796	-1.88952
C	2.09268	-0.84064	-2.79004
H	2.94095	-1.27631	-2.25363
C	2.30254	-1.06470	-4.28695
H	1.53206	-0.55154	-4.86679
H	2.22455	-2.13858	-4.48913
C	3.68939	-0.63257	-4.71576
O	4.66920	-0.77908	-3.97716
N	3.78980	-0.13987	-5.95964
H	4.69628	0.14507	-6.30894
H	2.97308	0.01270	-6.53519
C	2.11711	0.65568	-2.46884
O	2.56085	1.46594	-3.28550
N	1.72462	1.02378	-1.23553
H	1.40531	0.33893	-0.55615
C	1.95051	2.37845	-0.78654
H	2.93071	2.70788	-1.15599
C	0.90761	3.36936	-1.33941
H	-0.02273	3.30166	-0.76942
H	0.70142	3.11022	-2.38372
O	1.36119	4.70782	-1.22096
H	2.11606	4.81391	-1.82330
C	1.98231	2.39773	0.73464
O	1.82302	1.37455	1.41114
N	2.19084	3.60153	1.28162
H	2.26395	4.41528	0.67609
C	2.25452	3.76873	2.71804
H	3.13581	3.24848	3.11286
C	2.36915	5.25868	3.04603
H	1.48496	5.75987	2.62785
C	2.44520	5.50558	4.54369
H	2.64144	6.56640	4.72549
H	1.50427	5.24752	5.03997
H	3.25516	4.91850	4.98930
O	3.54195	5.71136	2.38359
H	3.57469	6.67609	2.48606
C	0.98468	3.22584	3.37209
O	-0.12935	3.58097	2.98176
N	1.17692	2.38701	4.40373
H	2.12832	2.15715	4.66554
C	0.09862	1.95420	5.27872
H	0.54740	1.23800	5.97450
C	-0.49919	3.11015	6.07729
H	-1.24608	2.73507	6.77852
H	0.29234	3.60705	6.64337
H	-0.97270	3.83701	5.41255
C	-0.99039	1.16074	4.55069
O	-2.08628	1.00698	5.09842
N	-0.66795	0.58974	3.37693
H	0.22629	0.79079	2.93422
C	-1.61853	-0.23080	2.64884
H	-2.33980	-0.60435	3.38025
C	-2.39481	0.55073	1.55424
H	-3.09631	-0.16681	1.10127
C	-3.21258	1.67170	2.19479
H	-3.83711	1.28905	3.00713
H	-2.55406	2.44803	2.60260
H	-3.86975	2.13927	1.45641
C	-1.49169	1.07372	0.42907
H	-0.96813	0.23297	-0.04554
H	-0.71574	1.72381	0.85738
C	-2.27902	1.83685	-0.63855
H	-2.52013	2.85452	-0.31604
H	-1.71165	1.90438	-1.57223
H	-3.22588	1.32952	-0.86167
C	-0.86056	-1.39704	2.03296
O	0.30853	-1.26864	1.64868

cis **c(KSTAIPF), conformation 9, 22 %**

N	-3.62057	-2.00403	-0.54860
C	-4.25534	-3.29774	-0.86183
H	-3.50502	-4.00808	-1.21986
H	-4.99458	-3.15154	-1.65561
C	-4.90367	-3.71491	0.46072
H	-4.22003	-4.34313	1.03991
H	-5.82599	-4.27524	0.29938
C	-5.13886	-2.38476	1.18196
H	-6.01070	-1.87123	0.76632
H	-5.26539	-2.48009	2.26172
C	-3.88083	-1.57435	0.82200
H	-4.06518	-0.50074	0.89059
C	-2.76727	-1.89536	1.81603
O	-2.85668	-1.47757	2.97251
N	-1.75126	-2.68304	1.40992
H	-1.68369	-2.96136	0.43539
C	-0.78841	-3.15952	2.38338
H	-1.33658	-3.36572	3.30780
C	-0.11235	-4.46691	1.94287
H	-0.90148	-5.20009	1.74958
H	0.46713	-4.82073	2.80069
C	0.78789	-4.33173	0.74051
C	0.30537	-4.56065	-0.55154
H	-0.73627	-4.84595	-0.68998
C	1.14584	-4.43785	-1.65693
H	0.75446	-4.61334	-2.65477
C	2.48771	-4.10570	-1.47966
H	3.14853	-4.02452	-2.33839
C	2.98073	-3.88186	-0.19397
H	4.02965	-3.63906	-0.04520
C	2.13357	-3.98495	0.90686
H	2.52131	-3.81689	1.91019
C	0.25280	-2.11534	2.78937
O	0.89541	-2.28561	3.83199
N	0.41598	-1.05073	1.99305
H	-0.07841	-0.98314	1.10417
C	1.29332	0.03854	2.38190
H	1.16675	0.20202	3.45720
C	2.77991	-0.25007	2.10756

H	3.37420	0.56316	2.54305
H	3.03721	-1.16565	2.65204
C	3.10951	-0.40104	0.62787
H	2.87870	0.52996	0.09753
H	2.48167	-1.18500	0.18409
C	4.58797	-0.71233	0.41024
H	5.18665	0.11719	0.80981
H	4.87577	-1.61790	0.95935
C	4.90639	-0.88632	-1.06442
H	4.49024	-0.07635	-1.66505
H	4.55862	-1.84335	-1.45654
N	6.38831	-0.84447	-1.27432
H	6.76060	0.07406	-1.00461
H	6.86196	-1.55657	-0.70612
H	6.63377	-1.00848	-2.25674
C	0.83386	1.28680	1.64179
O	0.12922	1.22088	0.62580
N	1.25970	2.46489	2.12060
H	1.85204	2.50333	2.94475
C	0.82964	3.70352	1.49612
H	-0.26409	3.75828	1.49878
C	1.37879	4.88941	2.27461
H	0.97542	4.86570	3.29364
H	1.04366	5.81072	1.78413
O	2.79300	4.78265	2.28353
H	3.14100	5.49765	2.83870
C	1.23854	3.80608	0.02496
O	0.53031	4.42380	-0.77035
N	2.40225	3.22343	-0.31688
H	2.96515	2.77980	0.40373
C	2.94434	3.26790	-1.65705
H	2.56348	4.16483	-2.15712
C	4.46971	3.35322	-1.59171
H	4.84668	3.27635	-2.61780
C	4.94767	4.64465	-0.95293
H	6.03963	4.63747	-0.87747
H	4.65173	5.50528	-1.55980
H	4.52862	4.76058	0.05144
O	4.87906	2.21735	-0.83174
H	5.83759	2.27677	-0.68769
C	2.50842	2.08297	-2.53350
O	2.97387	1.95801	-3.67016
N	1.58731	1.25954	-2.01549
H	1.26408	1.41420	-1.06302
C	1.03506	0.12058	-2.74948
H	0.64210	0.49161	-3.70282
C	2.04356	-0.98810	-2.99857
H	1.57367	-1.79323	-3.57205
H	2.89649	-0.60414	-3.56152
H	2.38972	-1.39907	-2.04873
C	-0.12859	-0.38424	-1.89253
O	-0.01890	-1.35101	-1.12986
N	-1.25445	0.33097	-1.98579
H	-1.29233	1.11715	-2.62439
C	-2.38319	0.04451	-1.12806
H	-2.00919	-0.01902	-0.09757
C	-3.42302	1.18279	-1.21239
H	-4.29953	0.85319	-0.64082
C	-2.86201	2.43830	-0.54002
H	-3.58946	3.25431	-0.57289
H	-2.62480	2.23922	0.51040
H	-1.94646	2.78299	-1.03584
C	-3.89233	1.44036	-2.65246
H	-4.05106	0.48162	-3.16011
H	-3.10827	1.96882	-3.21094
C	-5.17914	2.25908	-2.71340
H	-5.50283	2.39596	-3.74939
H	-5.98665	1.75354	-2.17298
H	-5.04963	3.25264	-2.27368
C	-2.96797	-1.32153	-1.51221
O	-2.85581	-1.77924	-2.65221

***trans* c(KSTAIPF), conformation 2, 33 %**

N	-3.93270	-0.70431	-0.31197
C	-4.75895	-1.30718	-1.37214
H	-4.16657	-2.02326	-1.95426
H	-5.15246	-0.54411	-2.04397
C	-5.85077	-2.00888	-0.56812
H	-6.32723	-2.81152	-1.13357
H	-6.61501	-1.28238	-0.27621
C	-5.10192	-2.51804	0.66549
H	-5.74858	-2.71284	1.52173
H	-4.56456	-3.43935	0.41880
C	-4.09002	-1.39291	0.96846
H	-4.45864	-0.69964	1.72906
C	-2.78278	-1.96922	1.48702
O	-2.59293	-2.09998	2.70037
N	-1.91155	-2.41339	0.56019
H	-2.06944	-2.21258	-0.42373
C	-0.72401	-3.15949	0.93909
H	-0.96586	-3.65427	1.88631
C	-0.34884	-4.22080	-0.09221
H	0.02956	-3.73916	-0.99933
H	-1.26040	-4.76860	-0.35317
C	0.67917	-5.17840	0.47311
C	1.99033	-5.21478	-0.00788
H	2.28102	-4.54167	-0.80986
C	2.92202	-6.10282	0.52829
H	3.93549	-6.12024	0.13881
C	2.55338	-6.96947	1.55606
H	3.27587	-7.66810	1.96914
C	1.24828	-6.93771	2.04819
H	0.94921	-7.61442	2.84426
C	0.32140	-6.04582	1.51140
H	-0.69748	-6.03091	1.89319
C	0.45405	-2.21750	1.21695
O	1.45129	-2.17041	0.50033
N	0.32231	-1.45700	2.33270
H	-0.48659	-1.66063	2.91601
C	1.52283	-0.97109	3.00400
H	1.17900	-0.46989	3.91598
C	2.48148	-2.10794	3.38702
H	2.95371	-2.50150	2.48020
H	3.27712	-1.68540	4.00743
C	1.78331	-3.24041	4.13288
H	0.93796	-3.61779	3.54186
H	1.36931	-2.86631	5.07847
C	2.73312	-4.40511	4.39930
H	3.08384	-4.81359	3.44181
H	3.61478	-4.06375	4.95560
C	2.03179	-5.49628	5.18523
H	1.12795	-5.84227	4.68009
H	1.77456	-5.17093	6.19409
N	2.92465	-6.68911	5.32937
H	3.81009	-6.43039	5.78025
H	2.48456	-7.42388	5.89450
H	3.14534	-7.08770	4.40836
C	2.24876	0.09666	2.19081
O	3.46234	0.27228	2.32915
N	1.50193	0.87668	1.38842
H	0.50307	0.72623	1.28408
C	2.11569	1.98875	0.70452
H	2.82158	2.47112	1.39123
C	2.92616	1.55887	-0.52806
H	2.26219	1.40729	-1.38745
H	3.43336	0.61352	-0.30136
O	3.86592	2.59246	-0.78686
H	4.13409	2.52910	-1.71626
C	1.04476	2.99853	0.31979
O	-0.16069	2.78266	0.49280
N	1.51458	4.12627	-0.22715
H	2.51400	4.21067	-0.39367
C	0.63046	5.18758	-0.65658
H	0.15955	5.65574	0.21642
C	1.44692	6.24268	-1.40624
H	1.92328	5.74625	-2.26328
C	0.58385	7.39566	-1.89057
H	0.02418	7.83353	-1.05750
H	1.22497	8.16791	-2.32605
H	-0.12263	7.07020	-2.66127
O	2.43872	6.68235	-0.48779
H	3.04224	7.26800	-0.97253
C	-0.43561	4.63649	-1.60035
O	-0.12410	3.94604	-2.57293
N	-1.69975	4.98777	-1.31036
H	-1.86188	5.58477	-0.50797
C	-2.81252	4.74154	-2.21276
H	-3.70968	5.06604	-1.67536
C	-2.69652	5.54065	-3.50824
H	-3.57411	5.36701	-4.13272

H	-2.63800	6.60633	-3.27467
H	-1.80362	5.24704	-4.06597
C	-3.05113	3.25626	-2.49483
O	-3.75398	2.94110	-3.45995
N	-2.55912	2.35974	-1.62062
H	-1.93874	2.65170	-0.86821
C	-2.85273	0.94624	-1.76128
H	-3.75645	0.88138	-2.36936
C	-1.73987	0.13544	-2.47569
H	-2.10463	-0.90248	-2.52192
C	-1.56187	0.64718	-3.90456
H	-1.14102	1.66014	-3.89988
H	-0.88353	0.00140	-4.46846
H	-2.51810	0.67622	-4.43504
C	-0.41507	0.13804	-1.70139
H	-0.58375	-0.22243	-0.67790
H	-0.05602	1.17372	-1.61650
C	0.65494	-0.73293	-2.35646
H	0.98514	-0.32272	-3.31547
H	1.53450	-0.82063	-1.71227
H	0.27127	-1.74513	-2.53572
C	-3.10807	0.35798	-0.38424
O	-2.52966	0.79229	0.62149

***cis* c(RSTAIPF), conformation 10, 34 %**

N	0.94244	3.10046	-2.52890
C	0.81889	4.56892	-2.58305
H	-0.04491	4.89664	-1.99899
H	0.66445	4.87521	-3.62271
C	2.15283	5.07061	-2.02449
H	2.07358	5.23762	-0.94586
H	2.46165	6.00674	-2.49245
C	3.11944	3.91766	-2.30834
H	3.41595	3.91195	-3.36107
H	4.01766	3.92807	-1.68926
C	2.25370	2.67719	-2.03521
H	2.62774	1.79977	-2.56867
C	2.28697	2.35176	-0.53920
O	3.34509	1.99872	-0.01128
N	1.15325	2.51616	0.16477
H	0.26909	2.61997	-0.32584
C	1.13737	2.25674	1.59230
H	1.92760	2.84812	2.06438
C	-0.23581	2.65853	2.15184
H	-1.00390	2.03015	1.68689
H	-0.41856	3.69076	1.83069
C	-0.34019	2.57385	3.65622
C	0.47005	3.36944	4.47502
H	1.21021	4.02578	4.02313
C	0.31348	3.35376	5.85921
H	0.93677	3.99015	6.48042
C	-0.64886	2.53035	6.44647
H	-0.77680	2.52404	7.52537
C	-1.44276	1.71529	5.64211
H	-2.18768	1.06404	6.09033
C	-1.29065	1.74362	4.25577
H	-1.92841	1.12663	3.62686
C	1.46170	0.79963	1.93051
O	2.18257	0.52669	2.90021
N	0.89306	-0.12619	1.15208
H	0.31293	0.16863	0.36619
C	1.10439	-1.54983	1.32503
H	2.05564	-1.69814	1.84432
C	-0.05269	-2.21853	2.09625
H	-0.97050	-2.05655	1.51693
H	0.12287	-3.30188	2.12657
C	-0.23889	-1.69179	3.51711
H	-1.21206	-2.02824	3.89122
H	-0.25749	-0.59523	3.52022
C	0.84264	-2.19130	4.47208
H	0.86846	-3.28329	4.47192
H	1.83754	-1.84842	4.17212
N	0.60397	-1.78076	5.85294
H	-0.02077	-2.35449	6.40941
C	0.95247	-0.60243	6.36685
N	1.68712	0.26474	5.67158
H	1.74931	0.20730	4.65420
H	1.80444	1.19248	6.06445
N	0.65645	-0.33314	7.64698
H	0.00049	-0.93376	8.13170
H	0.70933	0.62891	7.96078
C	1.16376	-2.17391	-0.06038
O	0.67754	-1.59323	-1.03903
N	1.67680	-3.40897	-0.16478
H	1.95983	-3.91642	0.66911
C	1.53708	-4.14102	-1.41191
H	2.05434	-3.61011	-2.21627
C	2.15478	-5.52284	-1.26161
H	3.22951	-5.41548	-1.07586
H	2.01203	-6.07158	-2.19981
O	1.51027	-6.16294	-0.17214
H	1.96940	-7.00096	-0.00527
C	0.07795	-4.26150	-1.86968
O	-0.19173	-4.30834	-3.06992
N	-0.85371	-4.34667	-0.90178
H	-0.56847	-4.35995	0.07378
C	-2.26907	-4.47950	-1.17237
H	-2.40675	-5.01854	-2.11483
C	-2.92644	-5.26725	-0.03703
H	-4.00395	-5.28499	-0.23710
C	-2.39447	-6.68423	0.07686
H	-2.86949	-7.18907	0.92391
H	-2.62019	-7.25218	-0.83039
H	-1.31149	-6.68673	0.23422
O	-2.65734	-4.50937	1.14156
H	-2.99607	-5.01052	1.90082
C	-2.99089	-3.13193	-1.31539
O	-4.20879	-3.10291	-1.50967
N	-2.22950	-2.03212	-1.22014
H	-1.24551	-2.13095	-0.98502
C	-2.79795	-0.69022	-1.16466
H	-3.56530	-0.61968	-1.94353
C	-3.40320	-0.38608	0.19773
H	-2.63189	-0.42081	0.97379
H	-3.85933	0.60718	0.20193
H	-4.17225	-1.12849	0.42452
C	-1.67115	0.28578	-1.50896
O	-1.30154	1.15969	-0.71421
N	-1.09273	0.13313	-2.70857
H	-1.35073	-0.66799	-3.27476
C	0.15882	0.81587	-2.98385
H	0.85839	0.55587	-2.17957
C	0.76568	0.36259	-4.33051
H	1.61377	1.03595	-4.51822
C	1.31373	-1.06081	-4.20891
H	2.05421	-1.12007	-3.40465
H	0.51789	-1.78445	-3.99263
H	1.80167	-1.36933	-5.13751
C	-0.21671	0.51943	-5.50052
H	-0.68975	1.50557	-5.44348
H	-1.02127	-0.22192	-5.40885
C	0.45485	0.36162	-6.86262
H	0.85175	-0.64743	-7.00751
H	-0.25890	0.55403	-7.66914
H	1.28458	1.06872	-6.97246
C	-0.07252	2.32720	-2.96914
O	-1.12526	2.82867	-3.37369

***trans* c(RSTAIPF), conformation 3, 64 %**

N	-2.10810	-3.39181	1.23500
C	-3.37557	-3.51590	1.97849
H	-3.61725	-2.59431	2.50995
H	-3.30050	-4.33354	2.70353
C	-4.37719	-3.84107	0.87232
H	-4.71916	-2.91515	0.39898
H	-5.24814	-4.37625	1.25415
C	-3.55396	-4.67641	-0.11260
H	-3.45623	-5.70258	0.25198
H	-3.97146	-4.70655	-1.12122
C	-2.16551	-4.01110	-0.08518
H	-1.35828	-4.73649	-0.20926
C	-1.99472	-3.00196	-1.21614
O	-1.59414	-3.38428	-2.32000
N	-2.35603	-1.72710	-0.97685
H	-2.64515	-1.44412	-0.04426
C	-2.32206	-0.72178	-2.02624
H	-2.50850	-1.24610	-2.96940
C	-3.39184	0.35065	-1.82540
H	-3.13960	0.95942	-0.95091
H	-4.34129	-0.15725	-1.62647

C	-3.51315	1.20678	-3.06607
C	-2.95268	2.48555	-3.13694
H	-2.44989	2.89546	-2.26548
C	-3.03540	3.23316	-4.31060
H	-2.59598	4.22561	-4.35011
C	-3.68258	2.71182	-5.43013
H	-3.74316	3.29378	-6.34647
C	-4.24784	1.43848	-5.36848
H	-4.75694	1.02534	-6.23567
C	-4.15933	0.69282	-4.19489
H	-4.59888	-0.30163	-4.14956
C	-0.92694	-0.08282	-2.11931
O	-0.69704	1.04194	-1.67194
N	0.01801	-0.83736	-2.72329
H	-0.30699	-1.71358	-3.12285
C	1.18288	-0.22767	-3.36001
H	1.69215	-1.04095	-3.88645
C	0.78718	0.85144	-4.38222
H	1.68920	1.10980	-4.94380
H	0.46222	1.75653	-3.85488
C	-0.31010	0.39018	-5.33371
H	-1.26294	0.27081	-4.79879
H	-0.05368	-0.58420	-5.76730
C	-0.49371	1.41833	-6.44034
H	0.42166	1.48098	-7.03838
H	-0.68666	2.40715	-6.00165
N	-1.60814	1.03929	-7.31017
H	-2.27763	0.37994	-6.92558
C	-2.07093	1.86808	-8.25098
N	-1.35224	2.92168	-8.62094
H	-0.44166	3.10021	-8.21901
H	-1.66944	3.51815	-9.37479
N	-3.25744	1.64798	-8.82019
H	-3.78684	0.81538	-8.59380
H	-3.53544	2.18504	-9.63150
C	2.20141	0.36183	-2.38800
O	3.08482	1.10002	-2.82861
N	2.11367	0.03045	-1.08335
H	1.33072	-0.52256	-0.74794
C	2.88078	0.77039	-0.10712
H	3.82547	1.05916	-0.57255
C	2.11803	2.04343	0.35142
H	2.83606	2.74382	0.78512
H	1.39794	1.77068	1.13399
O	1.47967	2.69646	-0.72342
H	0.77787	2.10344	-1.05831
C	3.14175	-0.08825	1.11442
O	2.48152	-1.10446	1.35729
N	4.08440	0.37332	1.94584
H	4.64570	1.17858	1.68874
C	4.37118	-0.28023	3.20514
H	4.90837	-1.22006	3.02729
C	5.25725	0.64435	4.04548
H	4.70258	1.57847	4.20950
C	5.63618	0.02430	5.37968
H	6.09667	-0.95788	5.23134
H	6.35482	0.67445	5.88757
H	4.76264	-0.08634	6.02992
O	6.40333	0.89621	3.24270
H	6.93101	1.57180	3.69761
C	3.07484	-0.55308	3.96864
O	2.22867	0.32775	4.12873
N	2.96243	-1.79811	4.46339
H	3.71896	-2.44915	4.29024
C	1.93692	-2.19861	5.41524
H	2.14183	-3.24850	5.64607
C	1.99555	-1.39812	6.71637
H	2.98742	-1.49919	7.16319
H	1.79122	-0.34019	6.53707
H	1.25674	-1.78640	7.41901
C	0.51458	-2.20132	4.85030
O	-0.41986	-2.39534	5.63536
N	0.34377	-2.06237	3.52393
H	1.13467	-1.86730	2.91252
C	-0.98896	-2.05208	2.94518
H	-1.63840	-2.57422	3.65121
C	-1.55196	-0.62148	2.73007
H	-2.55206	-0.74140	2.28658
C	-1.70343	0.08330	4.07886
H	-0.71876	0.30473	4.51030
H	-2.23991	1.02852	3.96313
H	-2.25889	-0.53612	4.78874
C	-0.70103	0.20055	1.75369
H	-0.63993	-0.31775	0.78748
H	0.32237	0.25515	2.14701
C	-1.24745	1.61070	1.53137
H	-2.31013	1.57811	1.26110
H	-1.15094	2.22677	2.43053
H	-0.71430	2.12038	0.72311
C	-0.96363	-2.79941	1.62398
O	0.04279	-2.81604	0.90469

cis **c(DSTAIPF), conformation 1, 49 %**

N	-2.07309	-3.19708	1.38477
C	-2.71326	-3.71718	2.60805
H	-2.33158	-3.18831	3.48603
H	-2.47024	-4.77916	2.71499
C	-4.20623	-3.48621	2.36775
H	-4.50952	-2.51741	2.77947
H	-4.81714	-4.26034	2.83480
C	-4.32609	-3.47436	0.84089
H	-4.28004	-4.49167	0.44206
H	-5.22990	-2.98924	0.46983
C	-3.05818	-2.71673	0.41426
H	-2.76951	-2.94768	-0.61385
C	-3.33044	-1.21167	0.49102
O	-4.17724	-0.70125	-0.24783
N	-2.65595	-0.50781	1.41293
H	-1.87935	-0.93930	1.90508
C	-2.90728	0.90515	1.60083
H	-3.98665	1.06064	1.69997
C	-2.19492	1.40432	2.87123
H	-2.45868	2.45830	3.00058
H	-1.11248	1.34237	2.71374
C	-2.59147	0.59611	4.08235
C	-1.79672	-0.46923	4.51642
H	-0.86210	-0.68614	4.00075
C	-2.19115	-1.25513	5.59879
H	-1.56199	-2.07839	5.92447
C	-3.38754	-0.98396	6.25928
H	-3.69467	-1.59282	7.10402
C	-4.18587	0.07746	5.83373
H	-5.11737	0.29761	6.34660
C	-3.79001	0.86020	4.75169
H	-4.41364	1.68797	4.42180
C	-2.46503	1.75761	0.41178
O	-3.02993	2.82831	0.17020
N	-1.41687	1.29988	-0.28915
H	-0.92407	0.46397	0.02263
C	-0.82944	2.07359	-1.36052
H	-1.62920	2.51640	-1.95947
C	0.08647	3.20221	-0.84298
H	0.93947	2.77687	-0.30162
H	-0.50058	3.81335	-0.14802
C	0.57850	4.09860	-1.98428
O	-0.26116	4.46165	-2.84075
O	1.81102	4.39726	-2.00863
C	0.00798	1.13121	-2.20931
O	0.41681	0.05350	-1.75899
N	0.36633	1.57225	-3.42467
H	0.08619	2.50724	-3.71733
C	1.40145	0.88560	-4.17716
H	1.05528	-0.10282	-4.49265
C	1.73817	1.71192	-5.41268
H	0.86751	1.73162	-6.07788
H	2.57161	1.23361	-5.94036
O	2.07237	3.01980	-4.97450
H	2.17322	3.57896	-5.76015
C	2.66627	0.63670	-3.34601
O	3.30100	-0.41133	-3.47467
N	3.05403	1.62887	-2.52297
H	2.52246	2.49994	-2.49482
C	4.27287	1.53487	-1.74596
H	5.06896	1.10495	-2.36267
C	4.70625	2.93192	-1.25787
H	5.62107	2.77664	-0.67770
C	5.00019	3.87931	-2.41210
H	4.12219	4.02920	-3.04772
H	5.30717	4.85091	-2.01524
H	5.81061	3.48383	-3.03138

O	3.74372	3.45342	-0.35582
H	2.98794	3.81909	-0.88136
C	4.14295	0.64914	-0.50792
O	5.15182	0.34853	0.13842
N	2.90380	0.28293	-0.15009
H	2.11261	0.61308	-0.69548
C	2.63406	-0.34065	1.14011
H	3.38826	-1.11840	1.29704
C	2.67867	0.67353	2.27340
H	2.47696	0.18826	3.23232
H	3.67146	1.12859	2.31324
H	1.93420	1.45808	2.11239
C	1.26193	-1.00414	1.03392
O	0.26455	-0.53012	1.59429
N	1.18767	-2.10358	0.27668
H	2.01577	-2.44120	-0.20094
C	-0.10456	-2.68976	-0.01672
H	-0.74260	-1.89805	-0.43220
C	0.02198	-3.81582	-1.06487
H	-0.98218	-4.25029	-1.16475
C	0.41868	-3.22424	-2.41953
H	0.44143	-4.00159	-3.18811
H	-0.29934	-2.46049	-2.73523
H	1.41263	-2.76070	-2.38418
C	0.96836	-4.93812	-0.61432
H	0.74226	-5.20847	0.42285
H	2.00496	-4.57536	-0.62542
C	0.86343	-6.18466	-1.48923
H	-0.16649	-6.55742	-1.51281
H	1.17297	-5.98667	-2.51972
H	1.50128	-6.98393	-1.10058
C	-0.72693	-3.19402	1.29167
O	-0.02714	-3.60538	2.22208

***trans* c(DSTAIPF), conformation 6, 61 %**

N	0.31891	-1.67290	-3.34157
C	0.88154	-2.78359	-4.12533
H	0.70727	-3.72660	-3.59576
H	1.95170	-2.66309	-4.28279
C	0.06431	-2.71751	-5.40984
H	0.11075	-3.64758	-5.97944
H	0.43587	-1.89976	-6.03504
C	-1.34091	-2.41461	-4.88678
H	-1.98398	-1.93032	-5.62315
H	-1.82667	-3.33921	-4.56604
C	-1.11768	-1.51460	-3.65830
H	-1.30098	-0.45701	-3.87850
C	-2.04753	-1.90329	-2.49452
O	-2.99411	-2.67180	-2.65428
N	-1.78209	-1.30310	-1.31287
H	-0.95808	-0.70505	-1.25229
C	-2.44779	-1.68848	-0.08338
H	-3.41890	-2.11570	-0.35985
C	-1.64244	-2.73835	0.70176
H	-2.14809	-2.91114	1.65507
H	-0.64807	-2.32648	0.91711
C	-1.54025	-4.02549	-0.07529
C	-0.49022	-4.25785	-0.96833
H	0.29324	-3.50996	-1.07945
C	-0.44688	-5.43066	-1.72293
H	0.38372	-5.60790	-2.40037
C	-1.46162	-6.37821	-1.60438
H	-1.42819	-7.28994	-2.19282
C	-2.51755	-6.15048	-0.72287
H	-3.31125	-6.88476	-0.62245
C	-2.55276	-4.98359	0.03562
H	-3.37615	-4.80790	0.72431
C	-2.73357	-0.46802	0.78574
O	-2.76503	-0.55768	2.02127
N	-2.96781	0.69267	0.15801
H	-2.86731	0.73376	-0.84967
C	-3.10269	1.93897	0.90842
H	-2.98995	2.74987	0.18533
C	-4.44286	2.10085	1.60695
H	-4.54991	1.37896	2.41976
H	-5.24004	1.90413	0.88060
C	-4.65070	3.52417	2.15185
O	-5.50539	3.65577	3.06555
O	-3.98651	4.45321	1.61864
C	-1.94064	2.06412	1.91019
O	-2.11056	2.40977	3.07789
N	-0.72783	1.80476	1.38114
H	-0.66879	1.45884	0.42723
C	0.47707	1.64140	2.16735
H	0.41249	2.27415	3.05553
C	0.64645	0.17210	2.58776
H	1.60993	0.04437	3.09151
H	0.64304	-0.44100	1.67657
O	-0.36433	-0.23793	3.48370
H	-1.18583	-0.37254	2.97184
C	1.64934	2.04969	1.28801
O	1.61948	1.83285	0.07107
N	2.70079	2.60582	1.90103
H	2.63742	2.86558	2.88047
C	3.81833	3.15253	1.15381
H	3.51845	4.09548	0.67874
C	4.96435	3.43742	2.12691
H	5.24246	2.48641	2.60051
C	6.16889	4.04367	1.42735
H	6.63462	3.32481	0.74545
H	5.87761	4.93433	0.86120
H	6.91460	4.33124	2.17424
O	4.42165	4.32404	3.09757
H	5.06559	4.39290	3.82034
C	4.31072	2.16699	0.09599
O	4.66950	1.02891	0.40491
N	4.37270	2.65968	-1.15264
H	4.03987	3.60289	-1.31024
C	5.02200	1.97986	-2.26187
H	4.89939	2.64165	-3.12485
C	6.51693	1.77247	-2.01643
H	6.68368	1.10442	-1.16795
H	6.98275	1.34012	-2.90295
H	6.98666	2.73713	-1.81005
C	4.35740	0.66647	-2.68316
O	4.95176	-0.04944	-3.49621
N	3.13228	0.37720	-2.20792
H	2.70023	0.96299	-1.49490
C	2.50750	-0.89311	-2.53478
H	2.95805	-1.21022	-3.47702
C	2.77381	-1.98797	-1.46813
H	2.29086	-2.90479	-1.83836
C	4.27115	-2.26233	-1.34147
H	4.71404	-2.49283	-2.31468
H	4.79208	-1.39325	-0.92213
H	4.44997	-3.11345	-0.67863
C	2.13852	-1.62405	-0.12100
H	1.06638	-1.42903	-0.26875
H	2.57704	-0.68427	0.24400
C	2.30296	-2.70958	0.94064
H	1.70114	-2.48328	1.82755
H	1.98151	-3.68613	0.55941
H	3.34373	-2.80110	1.26543
C	1.00506	-0.69630	-2.71794
O	0.43132	0.29780	-2.24404

***trans,trans* dimer of c(KSTAIPF)**

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ATOM      1  N   PRO     1      29.643  26.035  29.807  0.00  0.00           N
ATOM      2  CA  PRO     1      29.100  27.375  29.794  0.00  0.00           C
ATOM      3  C   PRO     1      28.606  27.874  28.439  0.00  0.00           C
ATOM      4  O   PRO     1      28.044  28.942  28.301  0.00  0.00           O
ATOM      5  CB  PRO     1      30.250  28.294  30.242  0.00  0.00           C
ATOM      6  CG  PRO     1      31.455  27.476  30.539  0.00  0.00           C
ATOM      7  CD  PRO     1      30.974  26.018  30.423  0.00  0.00           C
ATOM      8  HA  PRO     1      28.329  27.260  30.555  0.00  0.00           H
ATOM      9  HB2 PRO     1      29.920  28.743  31.178  0.00  0.00           H
ATOM     10  HB3 PRO     1      30.514  29.017  29.471  0.00  0.00           H
ATOM     11  HG2 PRO     1      32.388  27.667  30.010  0.00  0.00           H
ATOM     12  HG3 PRO     1      31.800  27.626  31.562  0.00  0.00           H
ATOM     13  HD2 PRO     1      31.633  25.542  29.697  0.00  0.00           H
ATOM     14  HD3 PRO     1      31.137  25.512  31.375  0.00  0.00           H
ATOM     15  N   PHE     2      28.766  27.056  27.301  0.00  0.00           N
ATOM     16  CA  PHE     2      28.178  27.328  25.963  0.00  0.00           C
ATOM     17  C   PHE     2      27.616  26.032  25.305  0.00  0.00           C
ATOM     18  O   PHE     2      28.242  24.981  25.491  0.00  0.00           O
ATOM     19  CB  PHE     2      29.255  28.051  25.155  0.00  0.00           C
ATOM     20  CG  PHE     2      30.592  27.301  24.996  0.00  0.00           C
ATOM     21  CD1 PHE     2      31.554  27.188  26.051  0.00  0.00           C
ATOM     22  CD2 PHE     2      30.848  26.586  23.818  0.00  0.00           C
ATOM     23  CE1 PHE     2      32.632  26.351  25.932  0.00  0.00           C
ATOM     24  CE2 PHE     2      32.030  25.859  23.616  0.00  0.00           C
ATOM     25  CZ  PHE     2      32.893  25.788  24.655  0.00  0.00           C
ATOM     26  H   PHE     2      29.091  26.100  27.339  0.00  0.00           H
ATOM     27  HA  PHE     2      27.318  27.979  26.124  0.00  0.00           H
ATOM     28  HB2 PHE     2      29.459  28.958  25.726  0.00  0.00           H
ATOM     29  HB3 PHE     2      28.872  28.453  24.217  0.00  0.00           H
ATOM     30  HD1 PHE     2      31.236  27.570  27.011  0.00  0.00           H
ATOM     31  HD2 PHE     2      30.078  26.611  23.062  0.00  0.00           H
ATOM     32  HE1 PHE     2      33.300  26.126  26.750  0.00  0.00           H
ATOM     33  HE2 PHE     2      32.208  25.249  22.743  0.00  0.00           H
ATOM     34  HZ  PHE     2      33.762  25.149  24.577  0.00  0.00           H
ATOM     35  N   LYS     3      26.538  26.168  24.422  0.00  0.00           N
ATOM     36  CA  LYS     3      25.948  25.229  23.399  0.00  0.00           C
ATOM     37  C   LYS     3      25.447  23.842  23.851  0.00  0.00           C
ATOM     38  O   LYS     3      24.467  23.268  23.361  0.00  0.00           O
ATOM     39  CB  LYS     3      26.945  25.117  22.272  0.00  0.00           C
ATOM     40  CG  LYS     3      26.541  24.118  21.110  0.00  0.00           C
ATOM     41  CD  LYS     3      27.263  24.112  19.763  0.00  0.00           C
ATOM     42  CE  LYS     3      26.887  22.883  18.889  0.00  0.00           C
ATOM     43  NZ  LYS     3      27.341  23.007  17.489  0.00  0.00           N1+
ATOM     44  H   LYS     3      26.106  27.080  24.404  0.00  0.00           H
ATOM     45  HA  LYS     3      25.033  25.627  22.963  0.00  0.00           H
ATOM     46  HB2 LYS     3      27.012  26.076  21.759  0.00  0.00           H
ATOM     47  HB3 LYS     3      27.881  24.896  22.785  0.00  0.00           H
ATOM     48  HG2 LYS     3      25.518  24.434  20.902  0.00  0.00           H
ATOM     49  HG3 LYS     3      26.463  23.104  21.500  0.00  0.00           H
ATOM     50  HD2 LYS     3      27.066  25.067  19.276  0.00  0.00           H
ATOM     51  HD3 LYS     3      28.339  24.130  19.935  0.00  0.00           H
ATOM     52  HE2 LYS     3      25.811  22.709  18.862  0.00  0.00           H
ATOM     53  HE3 LYS     3      27.421  22.043  19.331  0.00  0.00           H
ATOM     54  HZ1 LYS     3      26.880  23.777  17.027  0.00  0.00           H
ATOM     55  HZ2 LYS     3      28.333  23.115  17.322  0.00  0.00           H
ATOM     56  HZ3 LYS     3      27.002  22.142  17.091  0.00  0.00           H
ATOM     57  N   SER     4      26.122  23.232  24.838  0.00  0.00           N
ATOM     58  CA  SER     4      26.117  21.815  25.323  0.00  0.00           C
ATOM     59  C   SER     4      25.883  21.645  26.844  0.00  0.00           C
ATOM     60  O   SER     4      26.082  22.571  27.650  0.00  0.00           O
ATOM     61  CB  SER     4      27.394  21.035  24.993  0.00  0.00           C
ATOM     62  OG  SER     4      27.884  21.462  23.727  0.00  0.00           O
ATOM     63  H   SER     4      26.820  23.836  25.247  0.00  0.00           H
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ATOM     64  HA  SER     4      25.315  21.224  24.883  0.00  0.00           H
ATOM     65  HB2 SER     4      27.203  19.963  25.046  0.00  0.00           H
ATOM     66  HB3 SER     4      28.229  21.222  25.669  0.00  0.00           H
ATOM     67  HG  SER     4      28.386  22.261  23.906  0.00  0.00           H
ATOM     68  N   THR     5      25.636  20.425  27.216  0.00  0.00           N
ATOM     69  CA  THR     5      25.587  19.913  28.576  0.00  0.00           C
ATOM     70  C   THR     5      26.797  20.280  29.539  0.00  0.00           C
ATOM     71  O   THR     5      27.857  19.837  29.292  0.00  0.00           O
ATOM     72  CB  THR     5      25.523  18.358  28.616  0.00  0.00           C
ATOM     73  CG2 THR     5      25.091  17.881  30.014  0.00  0.00           C
ATOM     74  OG1 THR     5      24.682  17.642  27.647  0.00  0.00           O
ATOM     75  H   THR     5      25.621  19.698  26.515  0.00  0.00           H
ATOM     76  HA  THR     5      24.668  20.323  28.994  0.00  0.00           H
ATOM     77  HB  THR     5      26.553  18.007  28.550  0.00  0.00           H
ATOM     78  HG1 THR     5      24.826  16.712  27.836  0.00  0.00           H
ATOM     79 1HG2 THR     5      25.050  16.792  30.072  0.00  0.00           H
ATOM     80 2HG2 THR     5      25.752  18.204  30.817  0.00  0.00           H
ATOM     81 3HG2 THR     5      24.095  18.256  30.249  0.00  0.00           H
ATOM     82  N   ALA     6      26.547  20.933  30.662  0.00  0.00           N
ATOM     83  CA  ALA     6      27.545  21.216  31.698  0.00  0.00           C
ATOM     84  C   ALA     6      28.784  22.028  31.266  0.00  0.00           C
ATOM     85  O   ALA     6      29.778  22.320  31.939  0.00  0.00           O
ATOM     86  CB  ALA     6      28.024  19.940  32.454  0.00  0.00           C
ATOM     87  H   ALA     6      25.706  21.493  30.695  0.00  0.00           H
ATOM     88  HA  ALA     6      26.944  21.693  32.472  0.00  0.00           H
ATOM     89  HB1 ALA     6      28.826  20.050  33.184  0.00  0.00           H
ATOM     90  HB2 ALA     6      27.200  19.454  32.977  0.00  0.00           H
ATOM     91  HB3 ALA     6      28.483  19.292  31.709  0.00  0.00           H
ATOM     92  N   ILE     7      28.694  22.617  30.076  0.00  0.00           N
ATOM     93  CA  ILE     7      29.668  23.527  29.525  0.00  0.00           C
ATOM     94  C   ILE     7      28.950  24.927  29.543  0.00  0.00           C
ATOM     95  O   ILE     7      27.812  24.996  29.207  0.00  0.00           O
ATOM     96  CB  ILE     7      30.130  22.919  28.211  0.00  0.00           C
ATOM     97  CG1 ILE     7      30.929  21.562  28.419  0.00  0.00           C
ATOM     98  CG2 ILE     7      31.110  23.822  27.445  0.00  0.00           C
ATOM     99  CD1 ILE     7      31.383  20.890  27.173  0.00  0.00           C
ATOM    100  H   ILE     7      27.944  22.413  29.430  0.00  0.00           H
ATOM    101  HA  ILE     7      30.602  23.609  30.082  0.00  0.00           H
ATOM    102  HB  ILE     7      29.253  22.723  27.595  0.00  0.00           H
ATOM    103 2HG1 ILE     7      30.295  20.886  28.994  0.00  0.00           H
ATOM    104 3HG1 ILE     7      31.827  21.785  28.994  0.00  0.00           H
ATOM    105 1HG2 ILE     7      30.781  24.862  27.442  0.00  0.00           H
ATOM    106 2HG2 ILE     7      32.006  23.904  28.062  0.00  0.00           H
ATOM    107 3HG2 ILE     7      31.416  23.503  26.450  0.00  0.00           H
ATOM    108 1HD1 ILE     7      30.562  20.502  26.570  0.00  0.00           H
ATOM    109 2HD1 ILE     7      32.085  21.506  26.611  0.00  0.00           H
ATOM    110 3HD1 ILE     7      31.975  20.015  27.438  0.00  0.00           H
ATOM    111  N   PRO     8      27.750  25.957  33.714  0.00  0.00           N
ATOM    112  CA  PRO     8      28.808  25.059  34.210  0.00  0.00           C
ATOM    113  C   PRO     8      28.564  23.681  34.843  0.00  0.00           C
ATOM    114  O   PRO     8      29.498  22.990  35.156  0.00  0.00           O
ATOM    115  CB  PRO     8      29.600  25.983  35.150  0.00  0.00           C
ATOM    116  CG  PRO     8      29.371  27.365  34.655  0.00  0.00           C
ATOM    117  CD  PRO     8      27.918  27.328  34.223  0.00  0.00           C
ATOM    118  HA  PRO     8      29.399  24.863  33.315  0.00  0.00           H
ATOM    119  HB2 PRO     8      30.650  25.697  35.183  0.00  0.00           H
ATOM    120  HB3 PRO     8      29.169  25.888  36.148  0.00  0.00           H
ATOM    121  HG2 PRO     8      29.414  28.048  35.503  0.00  0.00           H
ATOM    122  HG3 PRO     8      30.093  27.541  33.857  0.00  0.00           H
ATOM    123  HD2 PRO     8      27.265  27.473  35.084  0.00  0.00           H
ATOM    124  HD3 PRO     8      27.716  28.129  33.511  0.00  0.00           H
ATOM    125  N   PHE     9      27.271  23.392  35.116  0.00  0.00           N
ATOM    126  CA  PHE     9      26.834  22.154  35.818  0.00  0.00           C
ATOM    127  C   PHE     9      25.496  21.579  35.290  0.00  0.00           C
ATOM    128  O   PHE     9      24.514  22.268  35.060  0.00  0.00           O
ATOM    129  CB  PHE     9      26.706  22.376  37.303  0.00  0.00           C
ATOM    130  CG  PHE     9      26.272  21.180  38.171  0.00  0.00           C
ATOM    131  CD1 PHE     9      24.952  20.936  38.597  0.00  0.00           C
ATOM    132  CD2 PHE     9      27.262  20.335  38.661  0.00  0.00           C
ATOM    133  CE1 PHE     9      24.624  19.906  39.502  0.00  0.00           C
ATOM    134  CE2 PHE     9      26.973  19.358  39.601  0.00  0.00           C
ATOM    135  CZ  PHE     9      25.671  19.098  40.001  0.00  0.00           C
ATOM    136  H   PHE     9      26.598  24.107  34.881  0.00  0.00           H
ATOM    137  HA  PHE     9      27.587  21.369  35.726  0.00  0.00           H
ATOM    138  HB2 PHE     9      25.907  23.110  37.404  0.00  0.00           H
ATOM    139  HB3 PHE     9      27.619  22.873  37.634  0.00  0.00           H
ATOM    140  HD1 PHE     9      24.138  21.517  38.191  0.00  0.00           H
ATOM    141  HD2 PHE     9      28.310  20.496  38.456  0.00  0.00           H
ATOM    142  HE1 PHE     9      23.610  19.808  39.859  0.00  0.00           H
ATOM    143  HE2 PHE     9      27.728  18.785  40.117  0.00  0.00           H
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ATOM    144  HZ  PHE     9      25.443  18.336  40.730  0.00  0.00           H
ATOM    145  N   LYS    10      25.463  20.263  34.937  0.00  0.00           N
ATOM    146  CA  LYS    10      24.264  19.461  34.551  0.00  0.00           C
ATOM    147  C   LYS    10      23.327  19.894  33.404  0.00  0.00           C
ATOM    148  O   LYS    10      22.629  19.004  32.911  0.00  0.00           O
ATOM    149  CB  LYS    10      23.527  19.063  35.874  0.00  0.00           C
ATOM    150  CG  LYS    10      22.191  18.292  35.726  0.00  0.00           C
ATOM    151  CD  LYS    10      21.586  17.991  37.077  0.00  0.00           C
ATOM    152  CE  LYS    10      20.557  16.864  36.968  0.00  0.00           C
ATOM    153  NZ  LYS    10      19.731  16.616  38.180  0.00  0.00           N1+
ATOM    154  H   LYS    10      26.322  19.735  35.001  0.00  0.00           H
ATOM    155  HA  LYS    10      24.644  18.544  34.102  0.00  0.00           H
ATOM    156  HB2 LYS    10      24.258  18.541  36.491  0.00  0.00           H
ATOM    157  HB3 LYS    10      23.247  19.960  36.426  0.00  0.00           H
ATOM    158  HG2 LYS    10      22.412  17.366  35.195  0.00  0.00           H
ATOM    159  HG3 LYS    10      21.443  18.850  35.162  0.00  0.00           H
ATOM    160  HD2 LYS    10      22.442  17.851  37.738  0.00  0.00           H
ATOM    161  HD3 LYS    10      21.071  18.877  37.449  0.00  0.00           H
ATOM    162  HE2 LYS    10      21.106  15.931  36.839  0.00  0.00           H
ATOM    163  HE3 LYS    10      19.918  17.110  36.120  0.00  0.00           H
ATOM    164  HZ1 LYS    10      19.219  17.432  38.483  0.00  0.00           H
ATOM    165  HZ2 LYS    10      18.997  15.997  37.868  0.00  0.00           H
ATOM    166  HZ3 LYS    10      20.209  16.288  39.007  0.00  0.00           H
ATOM    167  N   SER    11      23.334  21.139  32.904  0.00  0.00           N
ATOM    168  CA  SER    11      22.385  21.637  31.903  0.00  0.00           C
ATOM    169  C   SER    11      23.170  22.294  30.827  0.00  0.00           C
ATOM    170  O   SER    11      24.348  22.674  31.027  0.00  0.00           O
ATOM    171  CB  SER    11      21.298  22.527  32.512  0.00  0.00           C
ATOM    172  OG  SER    11      20.624  21.792  33.504  0.00  0.00           O
ATOM    173  H   SER    11      24.027  21.735  33.335  0.00  0.00           H
ATOM    174  HA  SER    11      21.893  20.809  31.394  0.00  0.00           H
ATOM    175  HB2 SER    11      20.630  22.869  31.722  0.00  0.00           H
ATOM    176  HB3 SER    11      21.688  23.438  32.968  0.00  0.00           H
ATOM    177  HG  SER    11      21.194  21.783  34.275  0.00  0.00           H
ATOM    178  N   THR    12      22.545  22.510  29.686  0.00  0.00           N
ATOM    179  CA  THR    12      23.095  23.246  28.568  0.00  0.00           C
ATOM    180  C   THR    12      23.475  24.608  28.972  0.00  0.00           C
ATOM    181  O   THR    12      22.838  25.396  29.603  0.00  0.00           O
ATOM    182  CB  THR    12      22.062  23.107  27.387  0.00  0.00           C
ATOM    183  CG2 THR    12      22.177  24.177  26.285  0.00  0.00           C
ATOM    184  OG1 THR    12      22.165  21.939  26.741  0.00  0.00           O
ATOM    185  H   THR    12      21.581  22.211  29.676  0.00  0.00           H
ATOM    186  HA  THR    12      23.990  22.689  28.292  0.00  0.00           H
ATOM    187  HB  THR    12      21.107  23.253  27.892  0.00  0.00           H
ATOM    188  HG1 THR    12      21.311  21.926  26.300  0.00  0.00           H
ATOM    189 1HG2 THR    12      21.609  23.932  25.386  0.00  0.00           H
ATOM    190 2HG2 THR    12      21.851  25.155  26.639  0.00  0.00           H
ATOM    191 3HG2 THR    12      23.224  24.257  25.986  0.00  0.00           H
ATOM    192  N   ALA    13      24.572  24.994  28.280  0.00  0.00           N
ATOM    193  CA  ALA    13      25.213  26.267  28.333  0.00  0.00           C
ATOM    194  C   ALA    13      25.456  26.891  29.721  0.00  0.00           C
ATOM    195  O   ALA    13      25.628  28.060  29.854  0.00  0.00           O
ATOM    196  CB  ALA    13      24.504  27.142  27.313  0.00  0.00           C
ATOM    197  H   ALA    13      25.065  24.263  27.788  0.00  0.00           H
ATOM    198  HA  ALA    13      26.214  26.152  27.918  0.00  0.00           H
ATOM    199  HB1 ALA    13      23.482  27.169  27.691  0.00  0.00           H
ATOM    200  HB2 ALA    13      24.909  28.153  27.351  0.00  0.00           H
ATOM    201  HB3 ALA    13      24.573  26.724  26.310  0.00  0.00           H
ATOM    202  N   ILE    14      25.490  26.096  30.753  0.00  0.00           N
ATOM    203  CA  ILE    14      25.869  26.469  32.127  0.00  0.00           C
ATOM    204  C   ILE    14      26.957  25.538  32.691  0.00  0.00           C
ATOM    205  O   ILE    14      26.997  24.342  32.366  0.00  0.00           O
ATOM    206  CB  ILE    14      24.702  26.630  33.075  0.00  0.00           C
ATOM    207  CG1 ILE    14      23.768  25.400  33.134  0.00  0.00           C
ATOM    208  CG2 ILE    14      24.018  27.975  32.623  0.00  0.00           C
ATOM    209  CD1 ILE    14      22.788  25.541  34.357  0.00  0.00           C
ATOM    210  H   ILE    14      25.398  25.102  30.599  0.00  0.00           H
ATOM    211  HA  ILE    14      26.461  27.374  31.984  0.00  0.00           H
ATOM    212  HB  ILE    14      25.144  26.777  34.061  0.00  0.00           H
ATOM    213 2HG1 ILE    14      24.385  24.524  33.339  0.00  0.00           H
ATOM    214 3HG1 ILE    14      23.254  25.218  32.190  0.00  0.00           H
ATOM    215 1HG2 ILE    14      24.657  28.851  32.519  0.00  0.00           H
ATOM    216 2HG2 ILE    14      23.390  27.729  31.765  0.00  0.00           H
ATOM    217 3HG2 ILE    14      23.399  28.246  33.479  0.00  0.00           H
ATOM    218 1HD1 ILE    14      22.311  24.566  34.464  0.00  0.00           H
ATOM    219 2HD1 ILE    14      23.392  25.538  35.264  0.00  0.00           H
ATOM    220 3HD1 ILE    14      22.119  26.402  34.382  0.00  0.00           H
END
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