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Article

A new general correlation for the influence parameter in density gradient theory and Peng-Robinson equation of state for *n*-alkanes

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Abstract: Supplementary material

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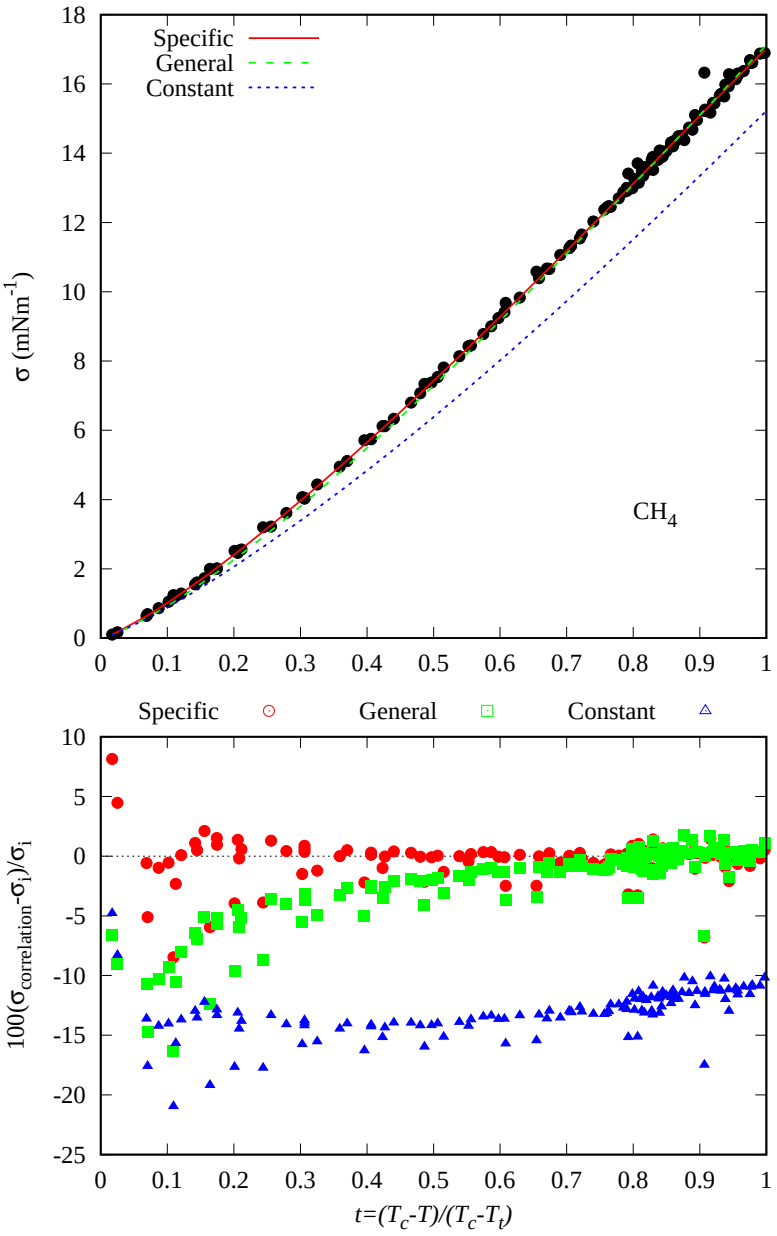

Figure 1. Surface tension data for methane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

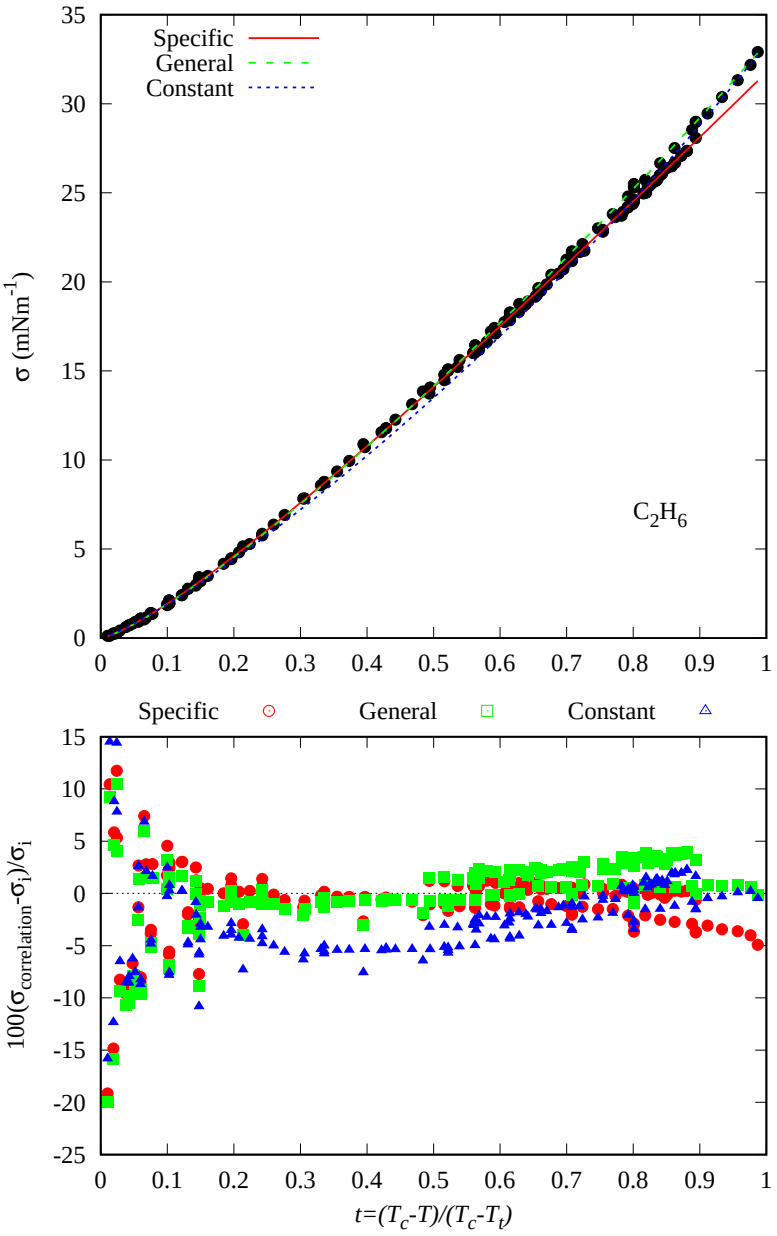

Figure 2. Surface tension data for ethane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

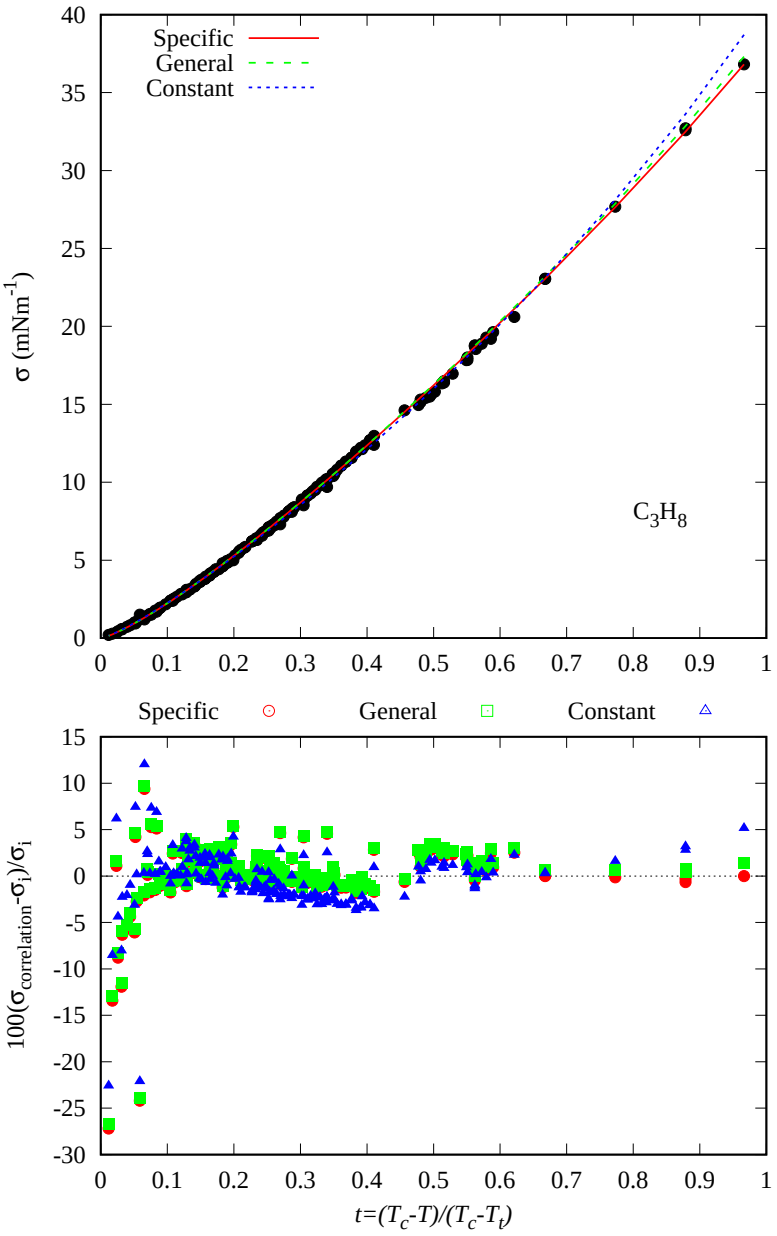

Figure 3. Surface tension data for propane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

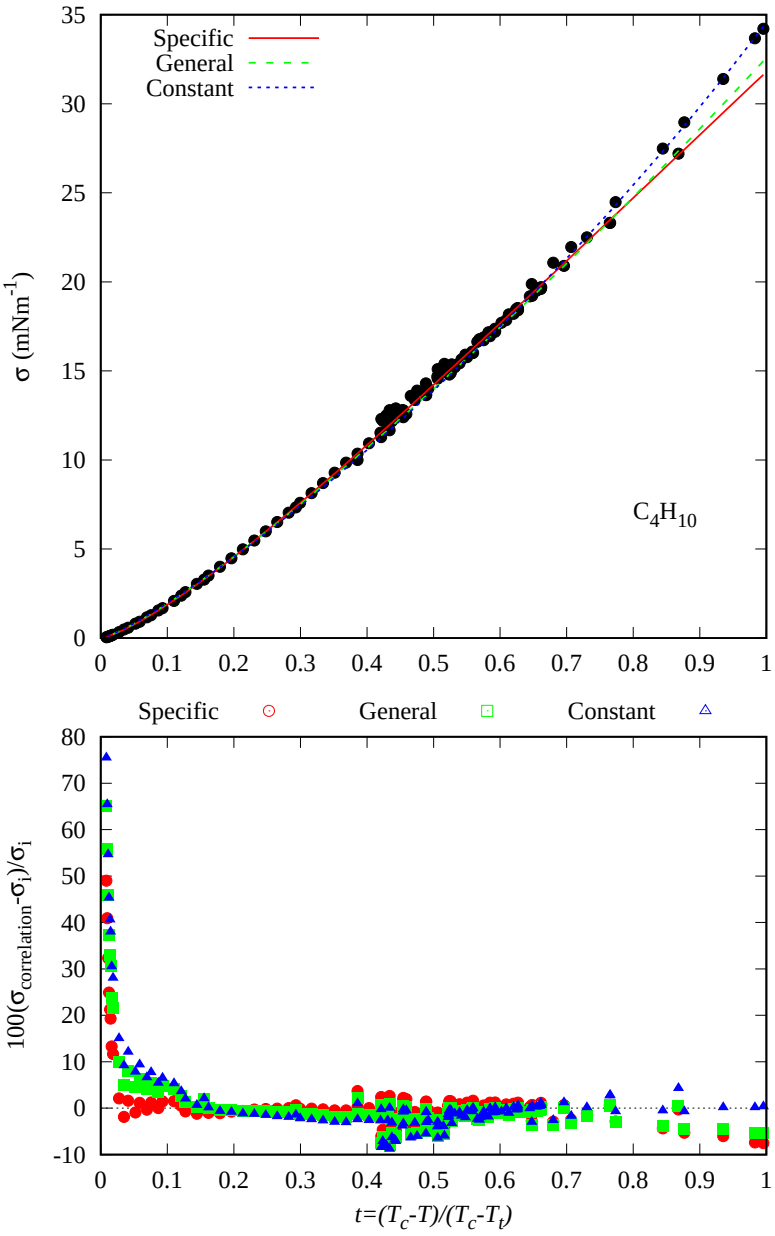

Figure 4. Surface tension data for *n*-butane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

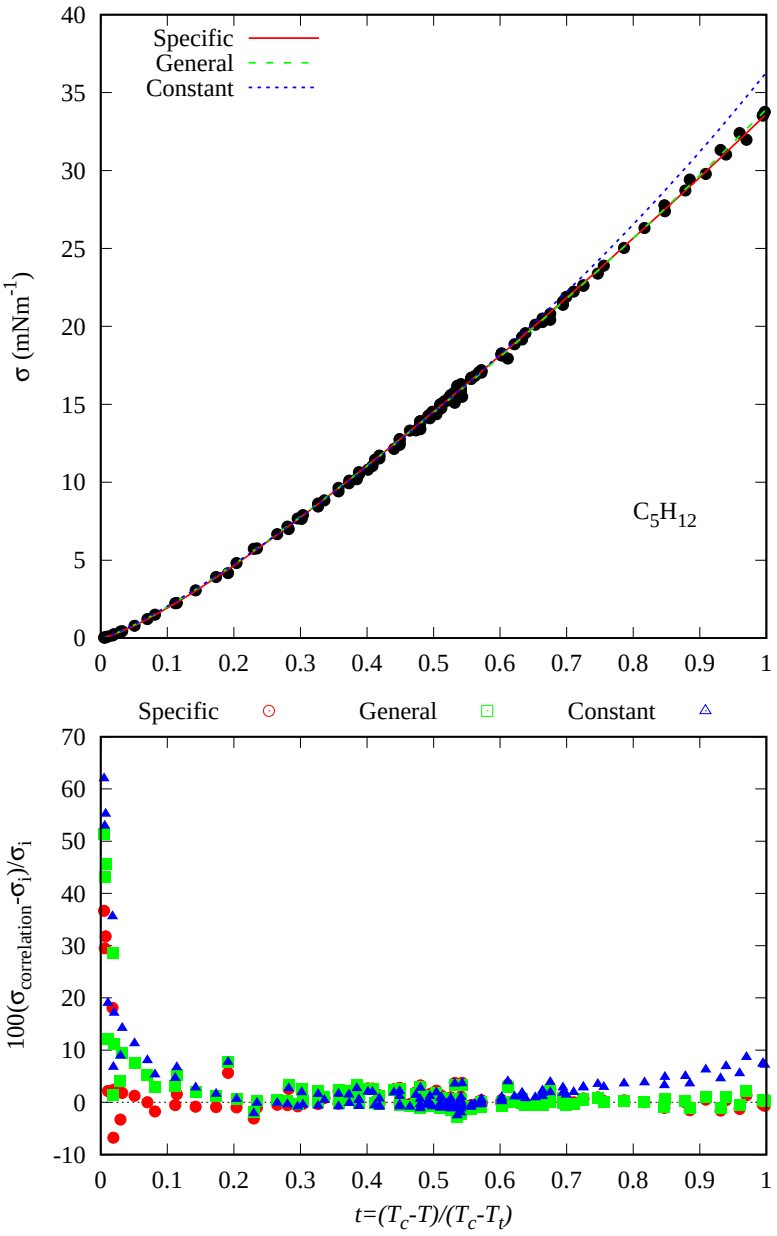

Figure 5. Surface tension data for *n*-pentane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

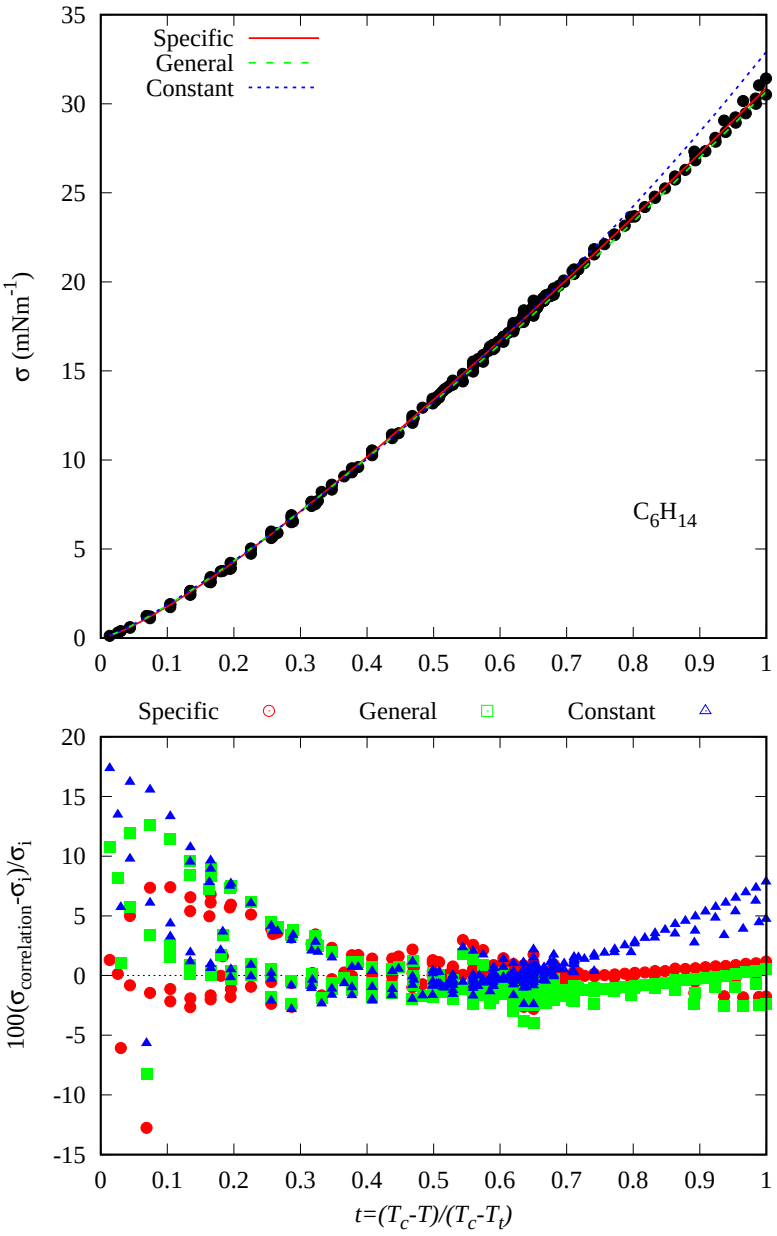

Figure 6. Surface tension data for *n*-hexane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

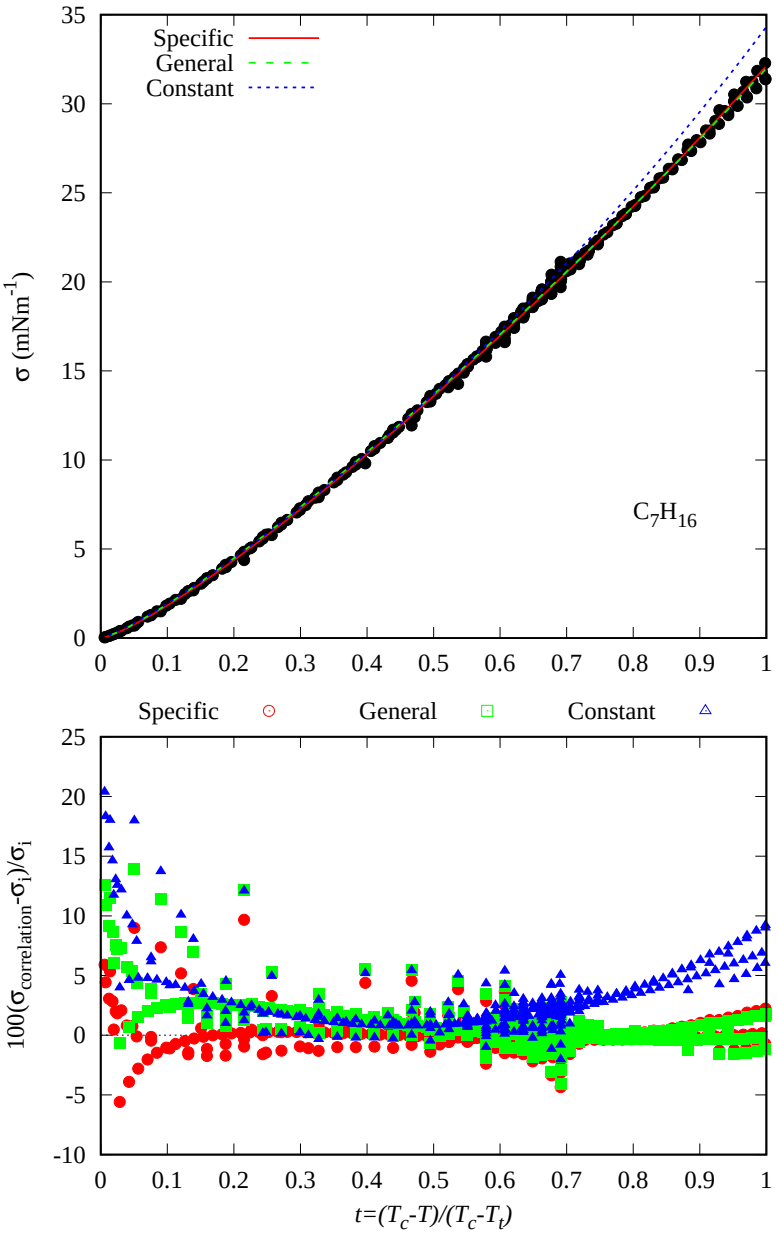

Figure 7. Surface tension data for *n*-heptane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

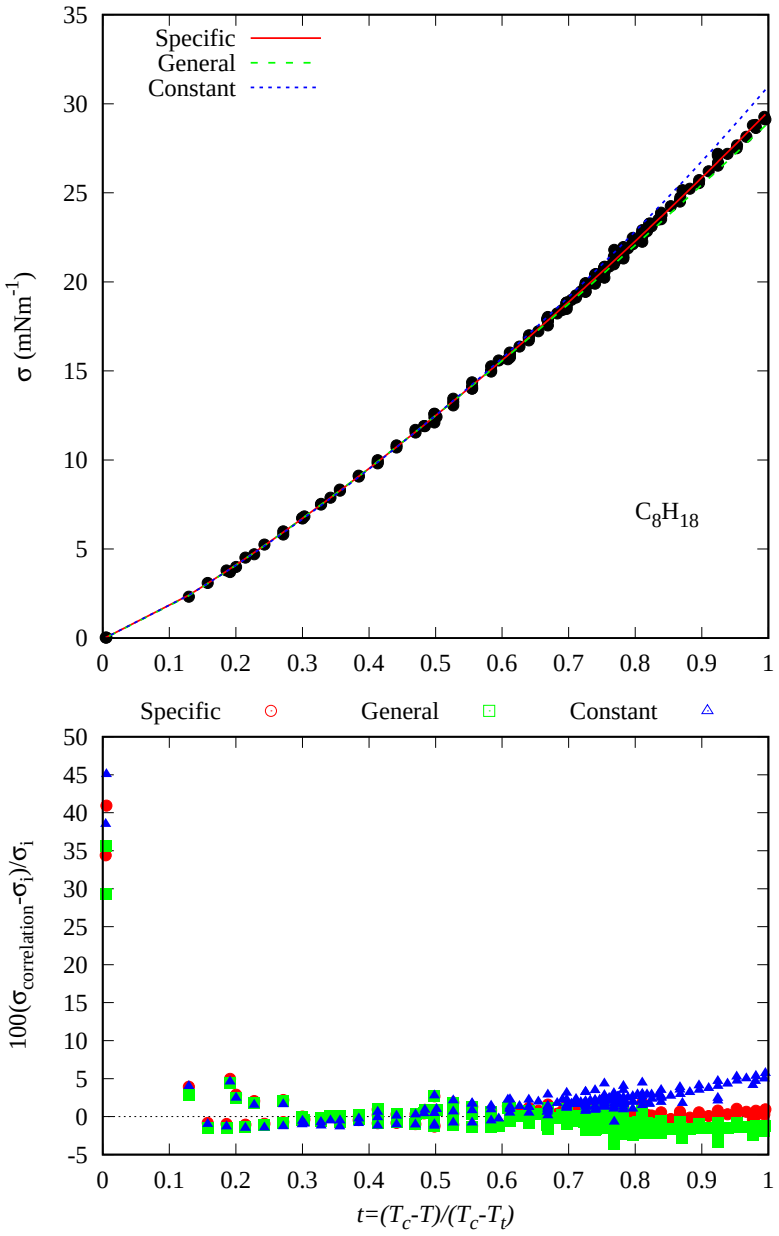

Figure 8. Surface tension data for *n*-octane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

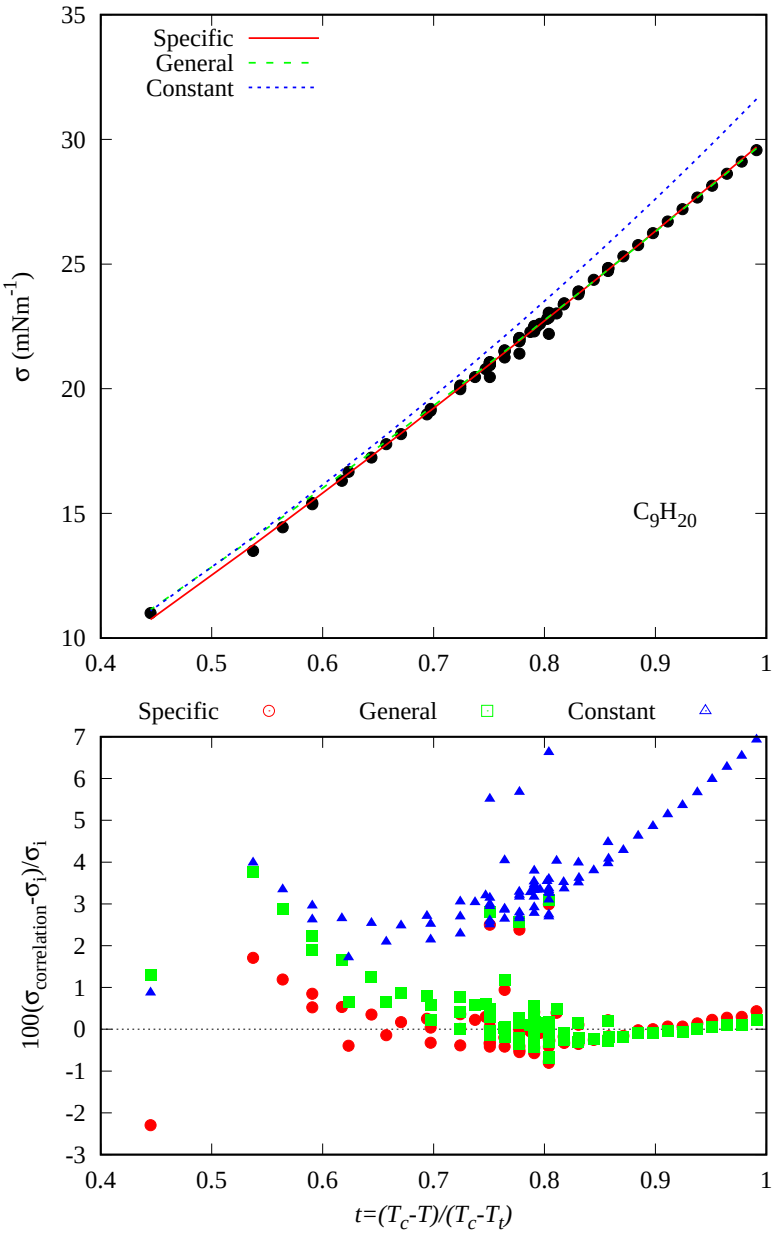

Figure 9. Surface tension data for *n*-nonane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

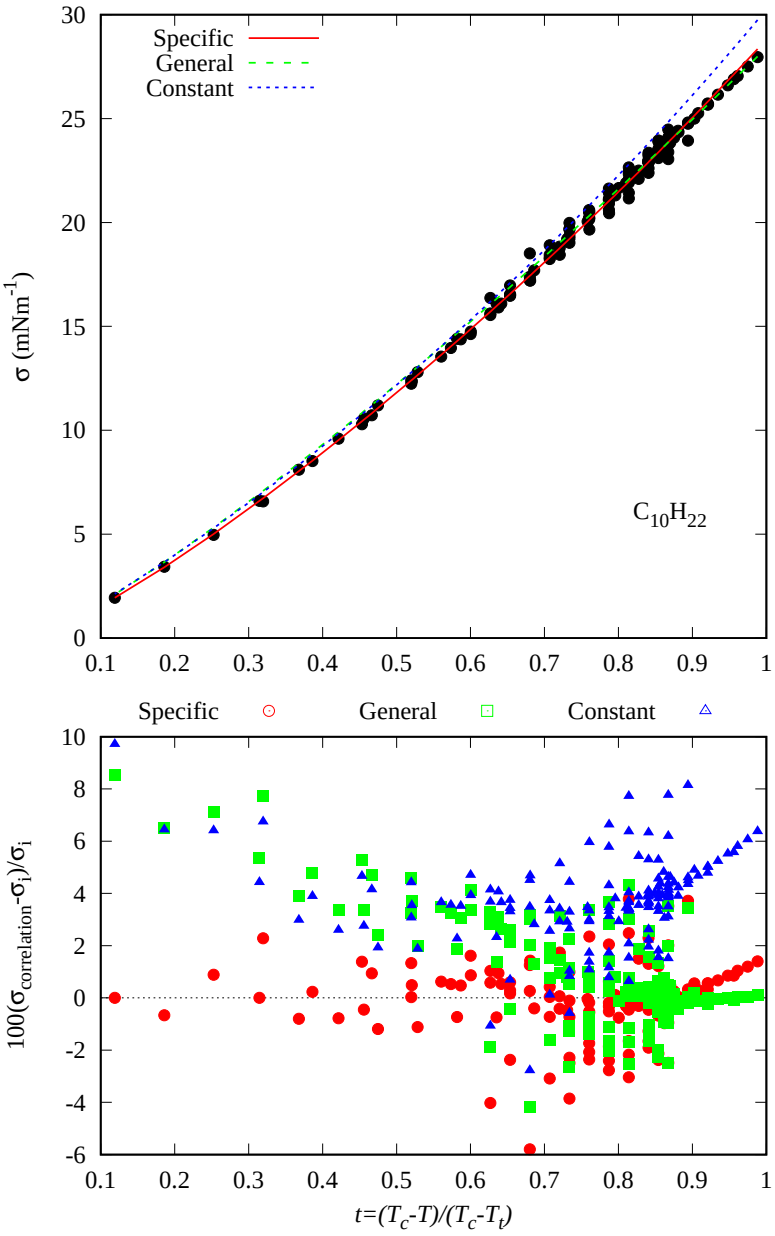

Figure 10. Surface tension data for *n*-decane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

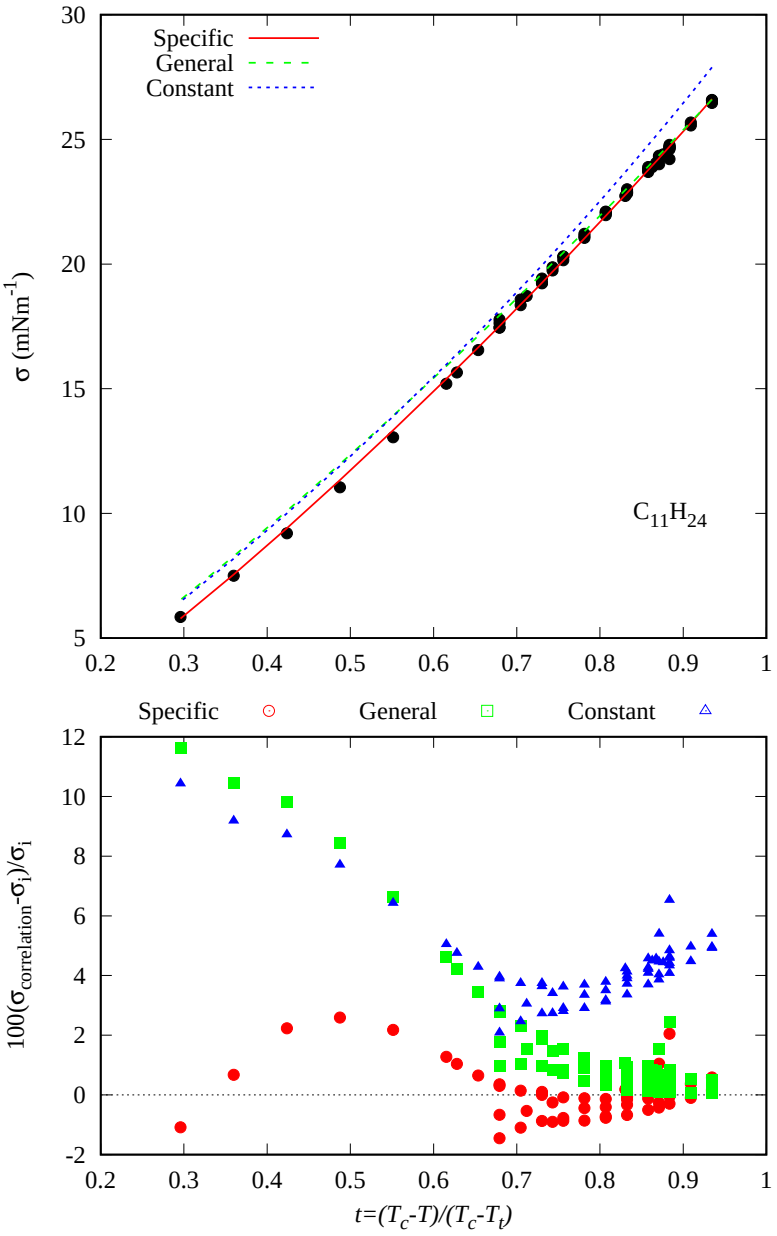

Figure 11. Surface tension data for *n*-undecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

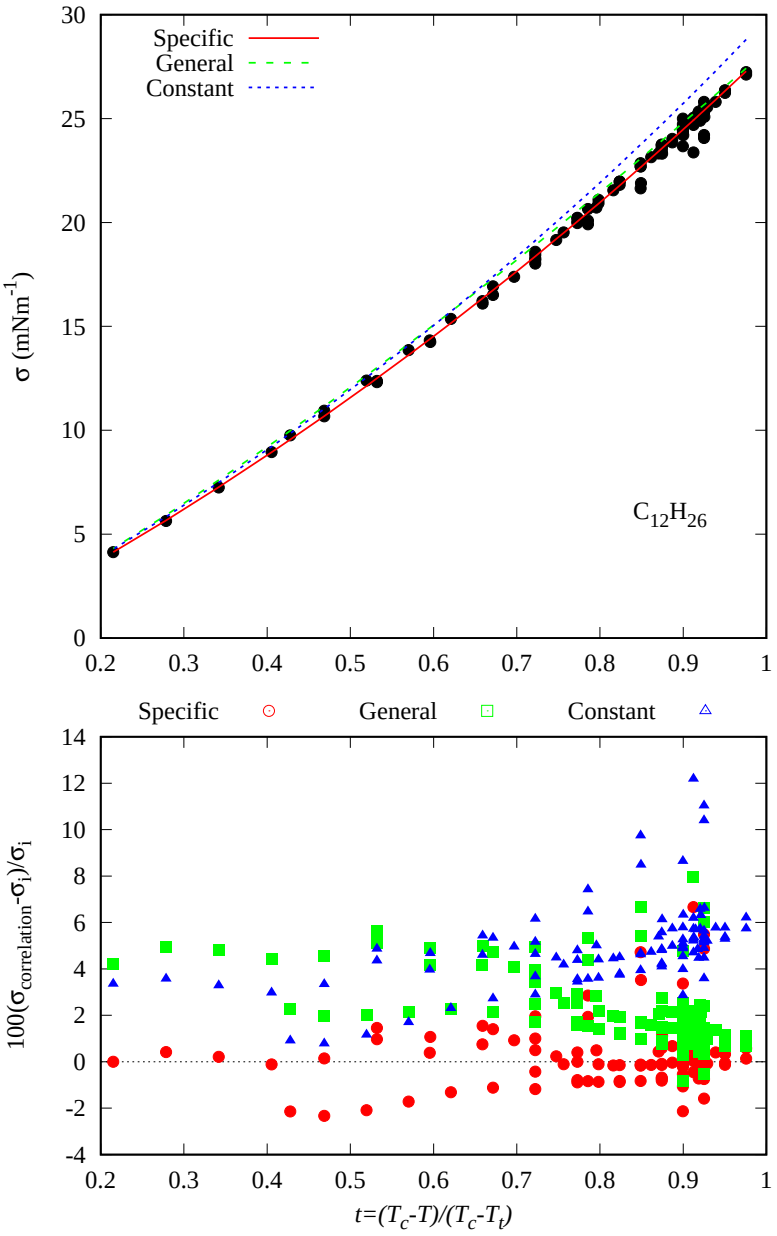

Figure 12. Surface tension data for *n*-dodecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

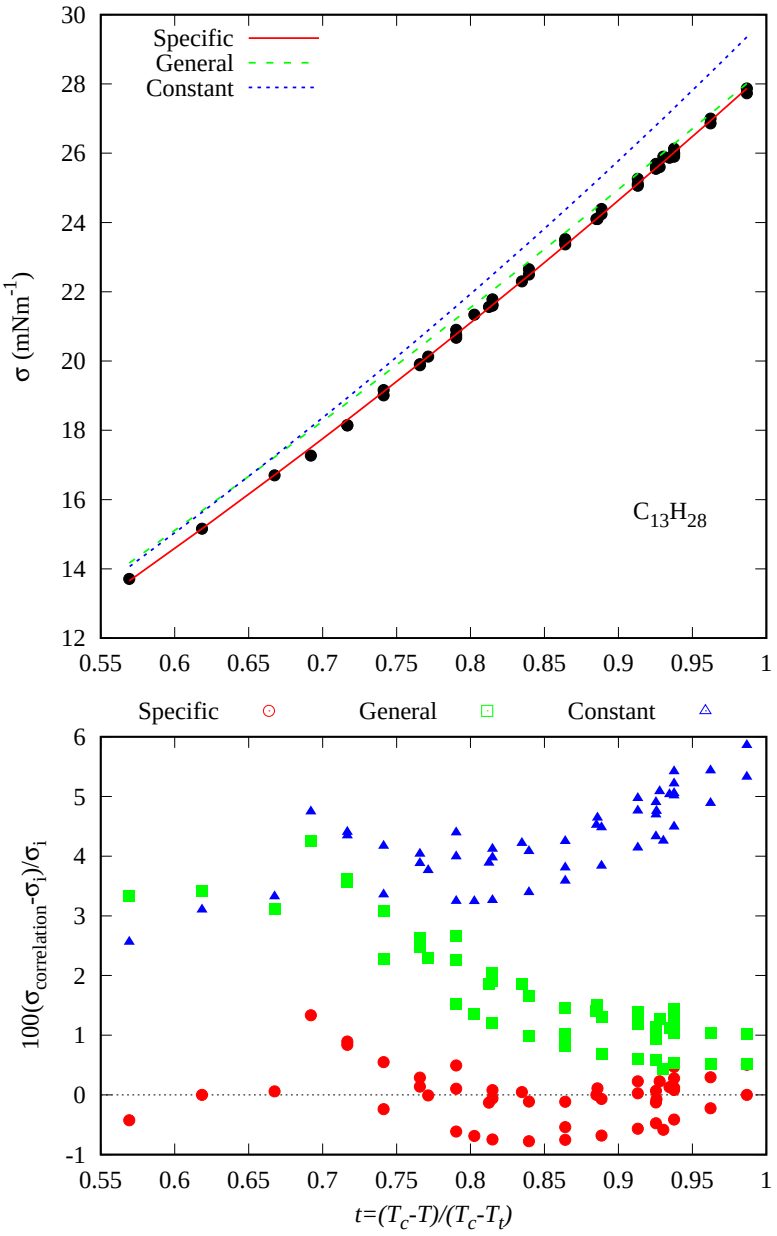

Figure 13. Surface tension data for *n*-tridecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

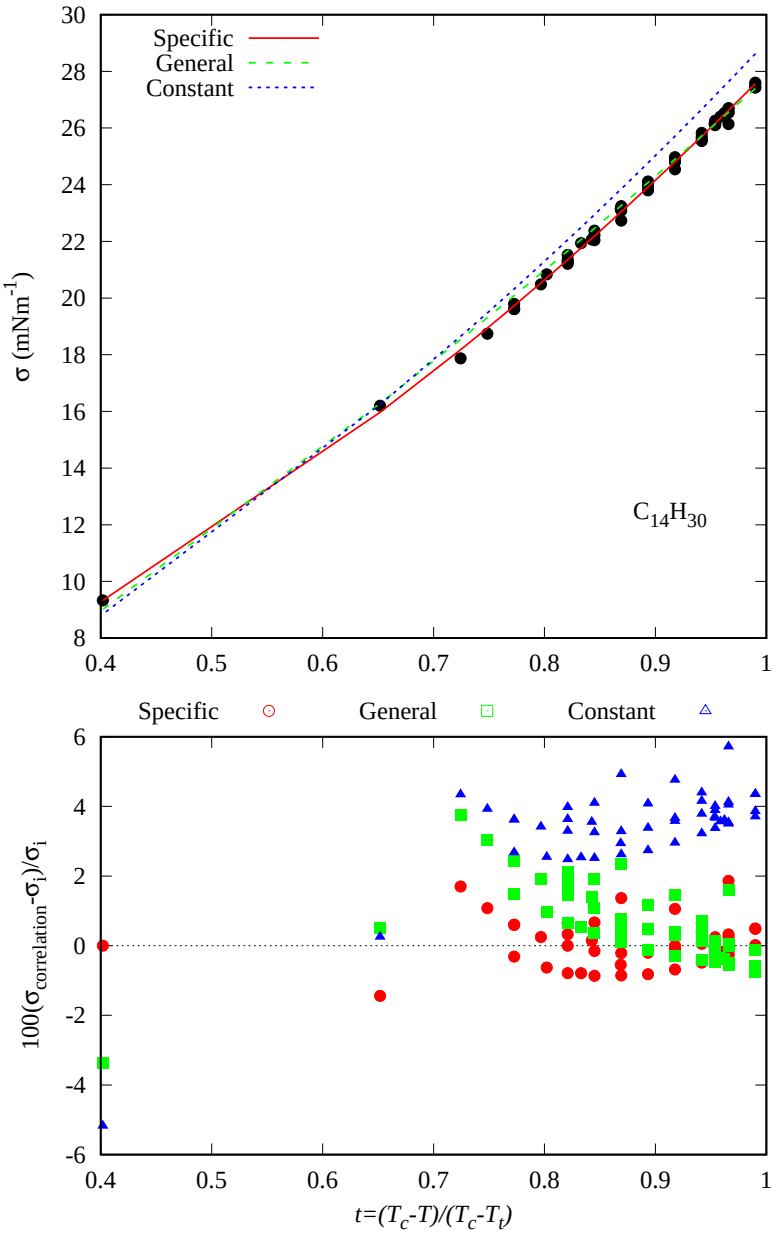

Figure 14. Surface tension data for *n*-tetradecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

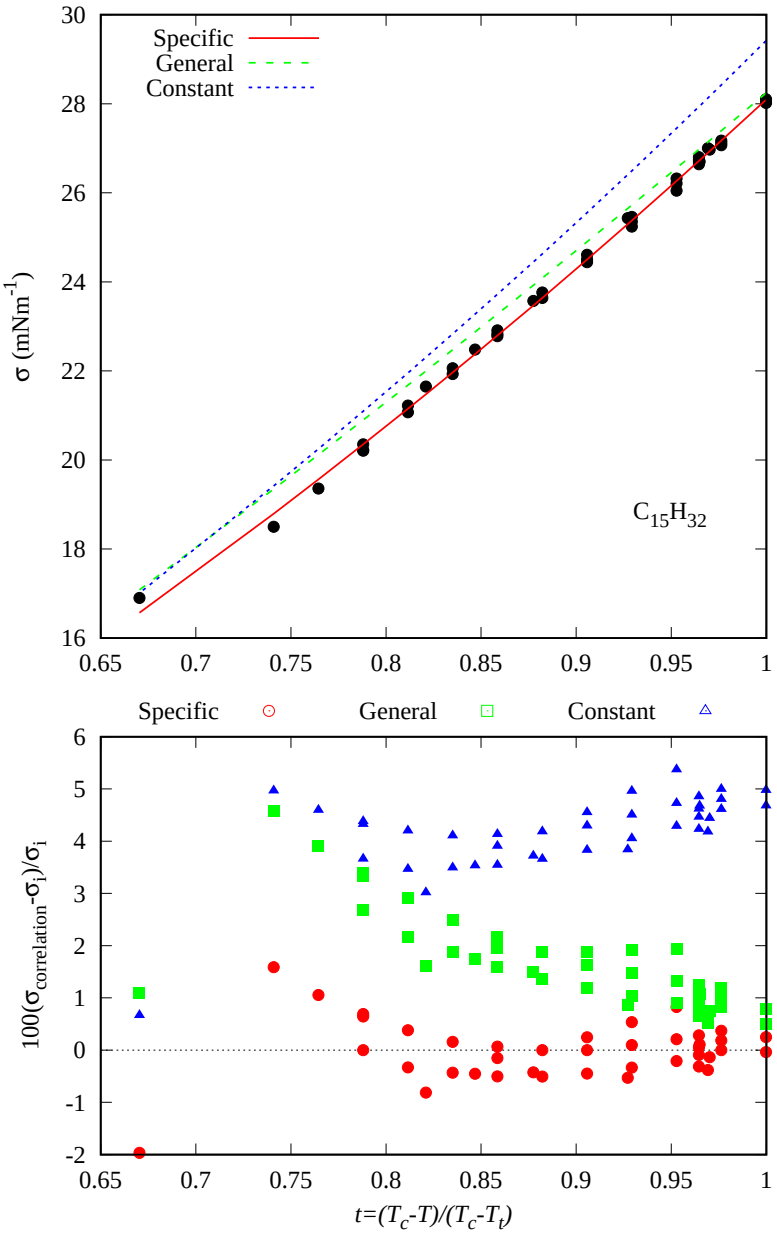

Figure 15. Surface tension data for *n*-pentadecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

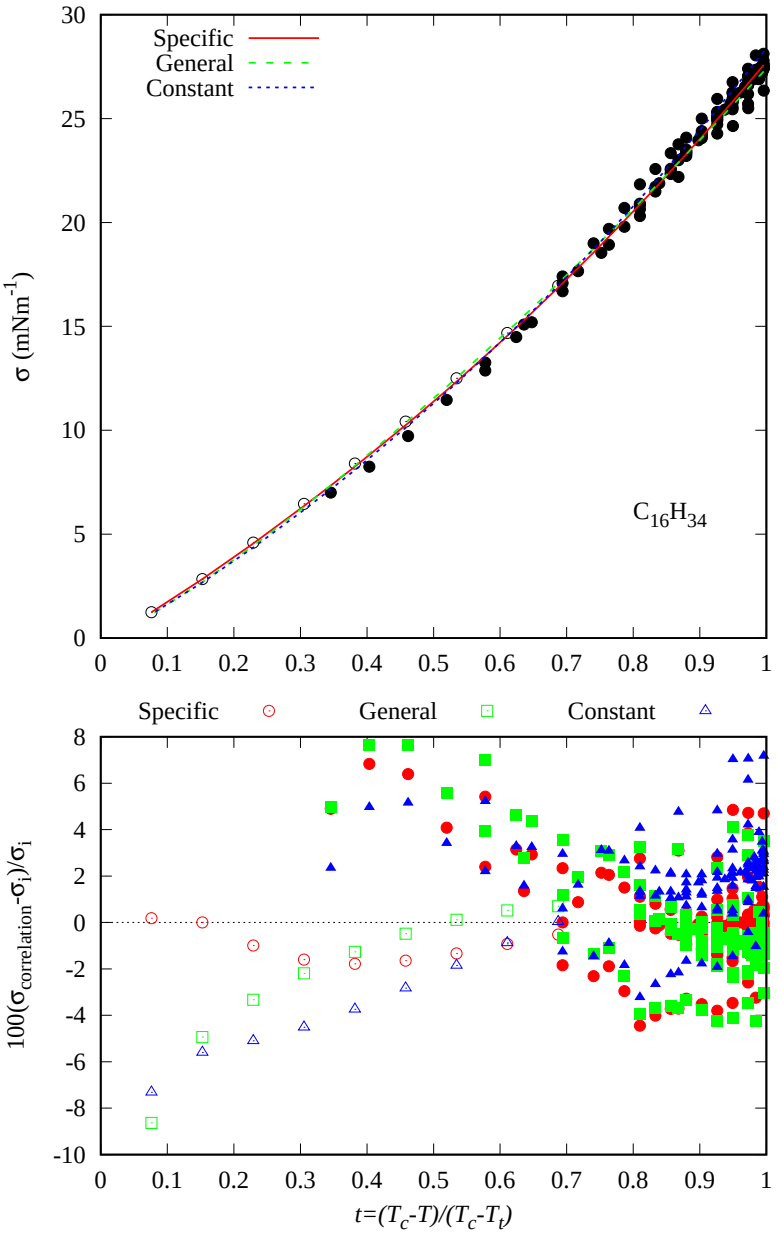

Figure 16. Surface tension data for *n*-hexadecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

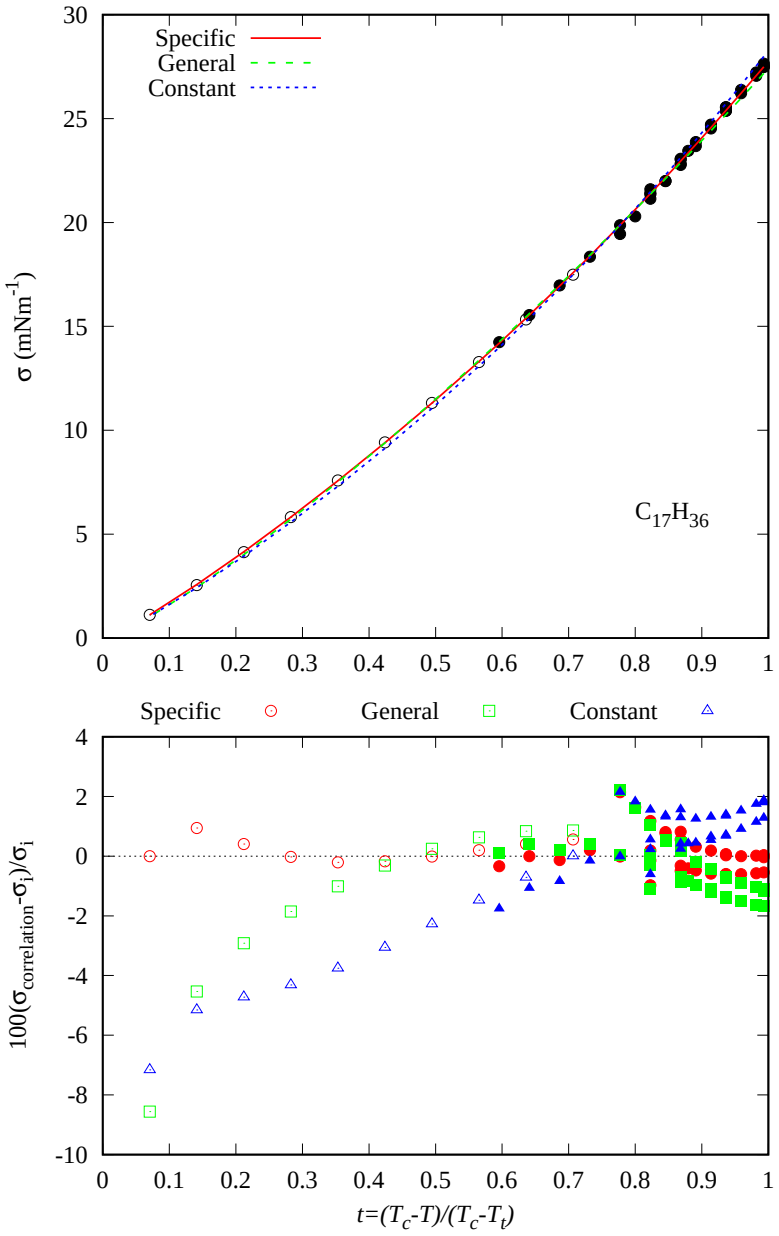

Figure 17. Surface tension data for *n*-heptadecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

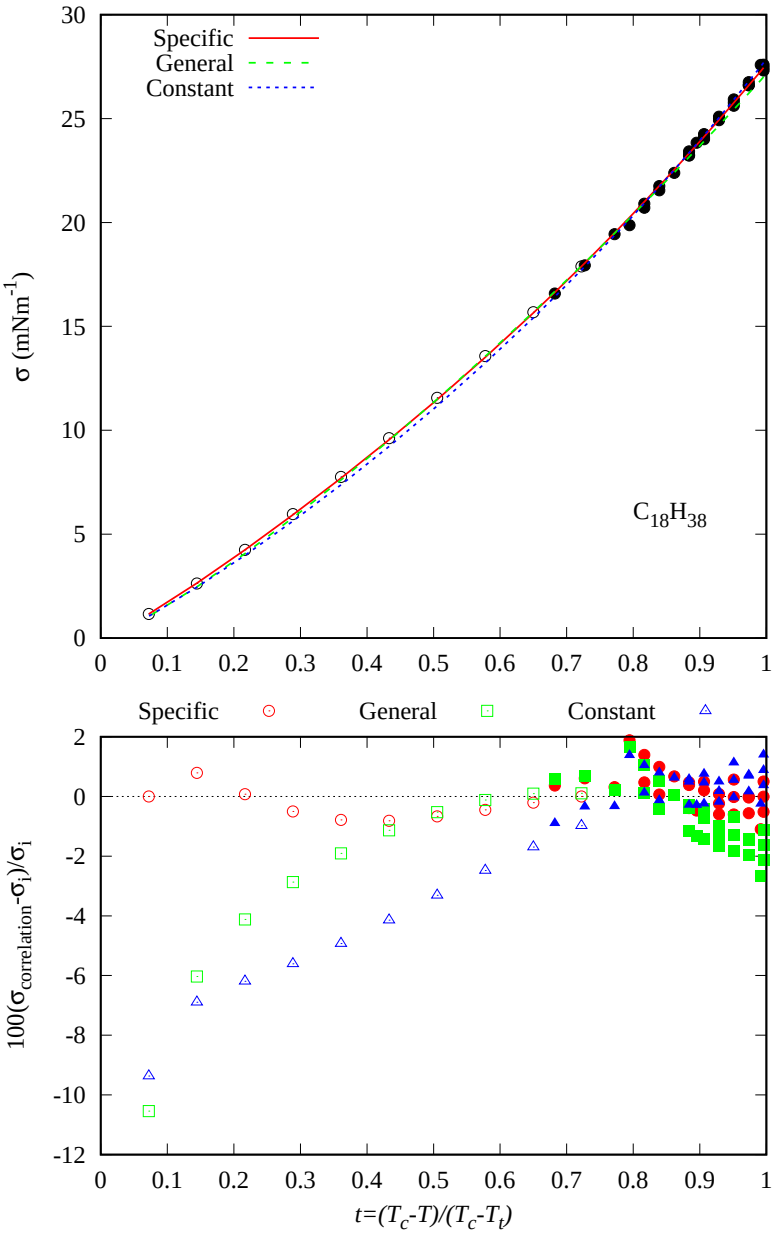

Figure 18. Surface tension data for *n*-octadecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

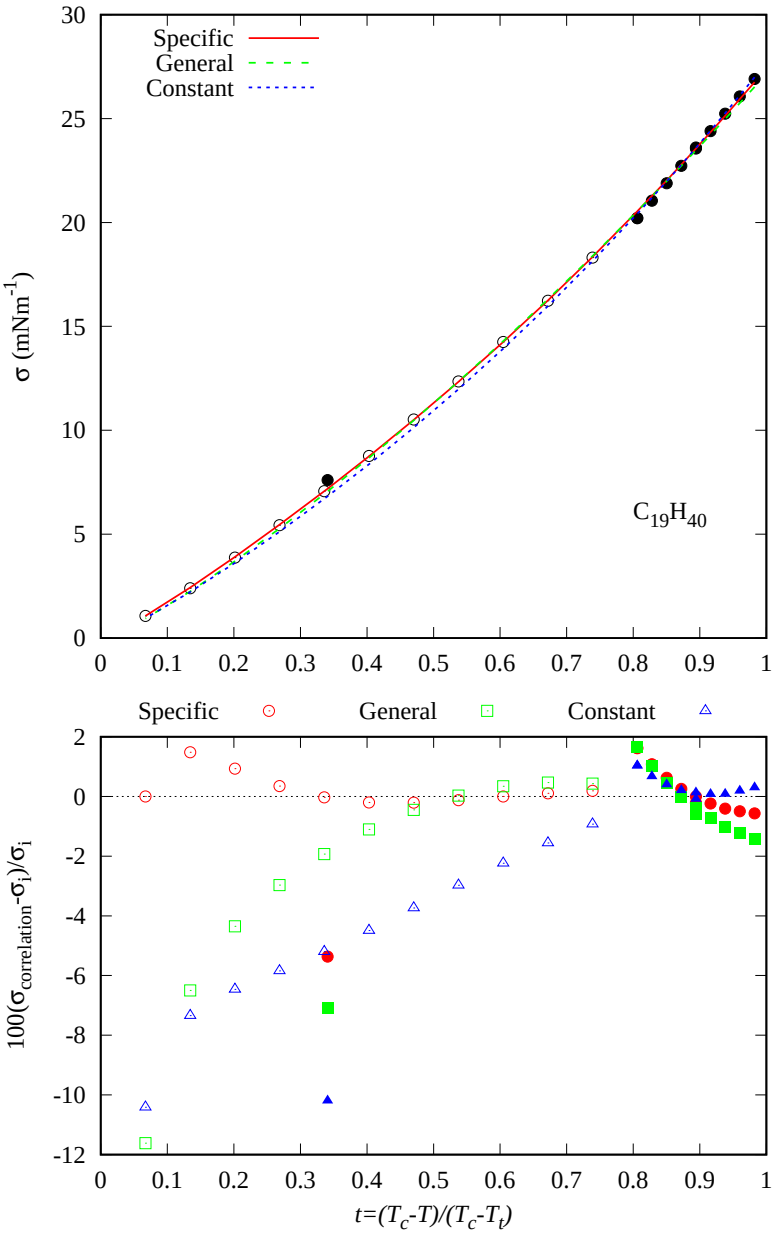

Figure 19. Surface tension data for *n*-nonadecane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

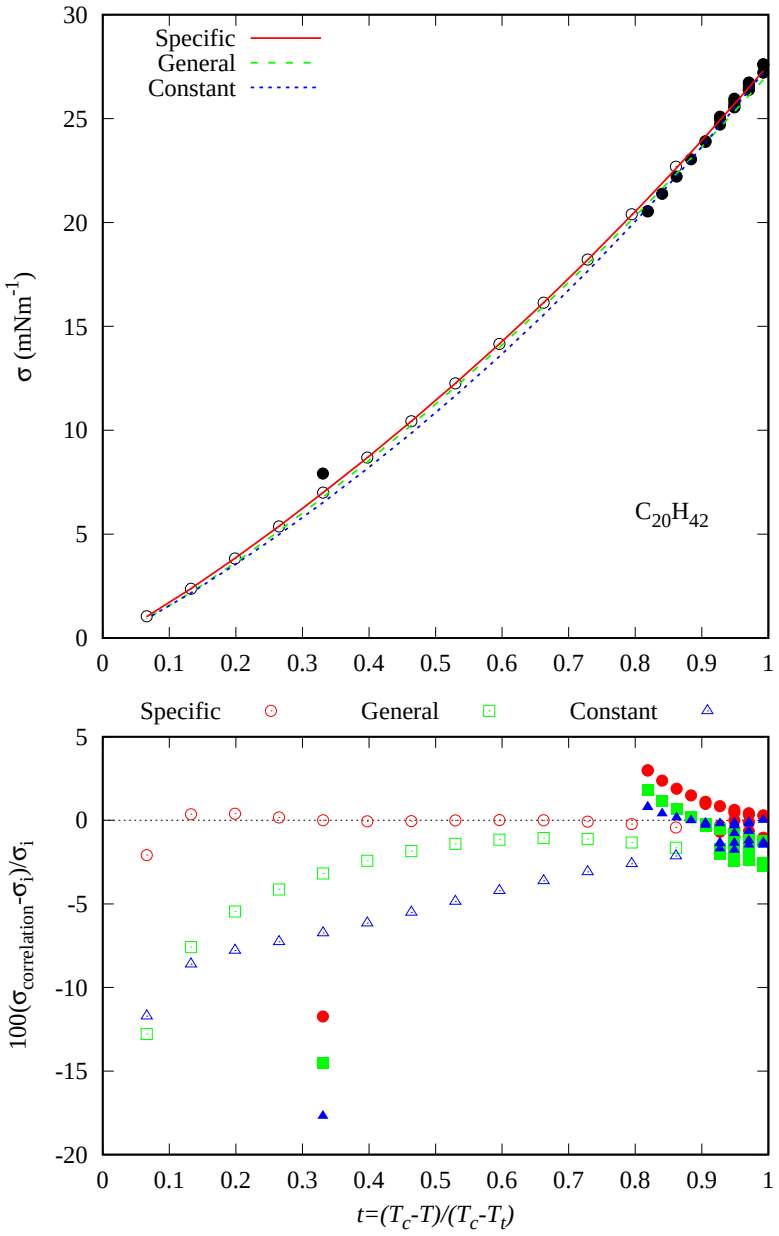

Figure 20. Surface tension data for *n*-eicosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

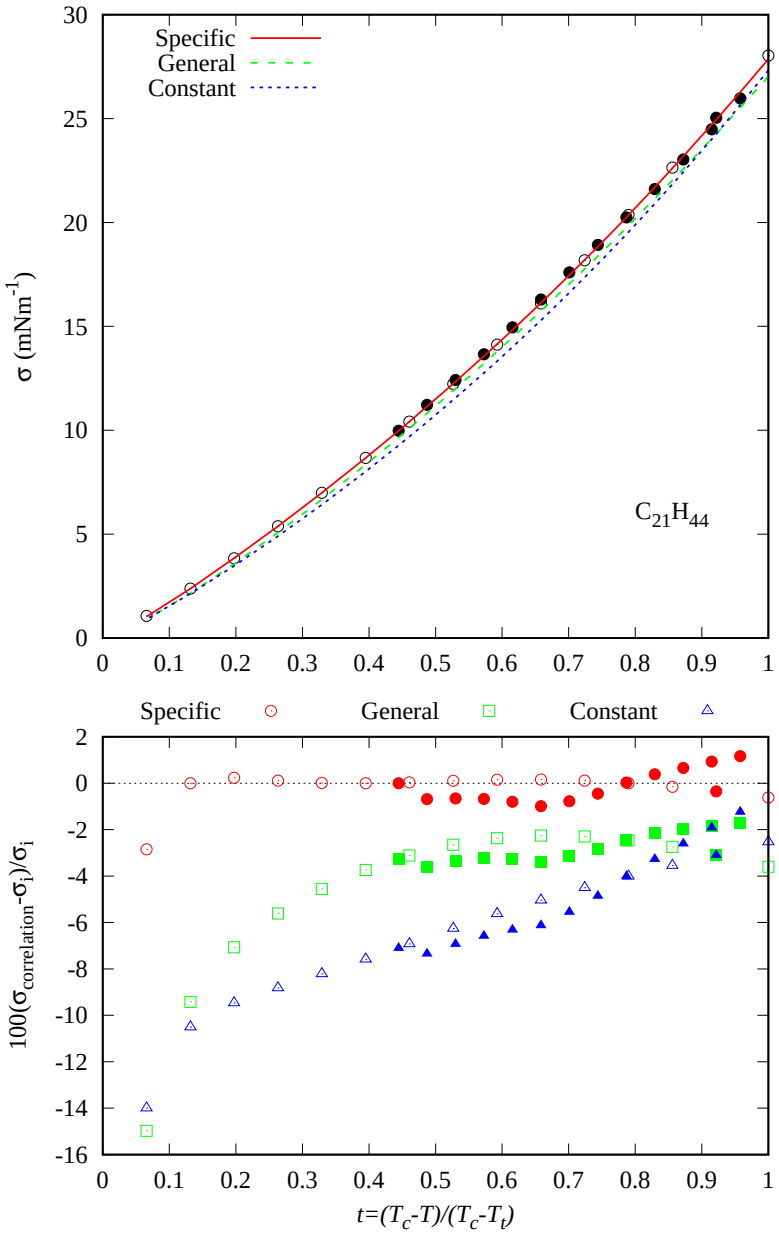

Figure 21. Surface tension data for *n*-heneicosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

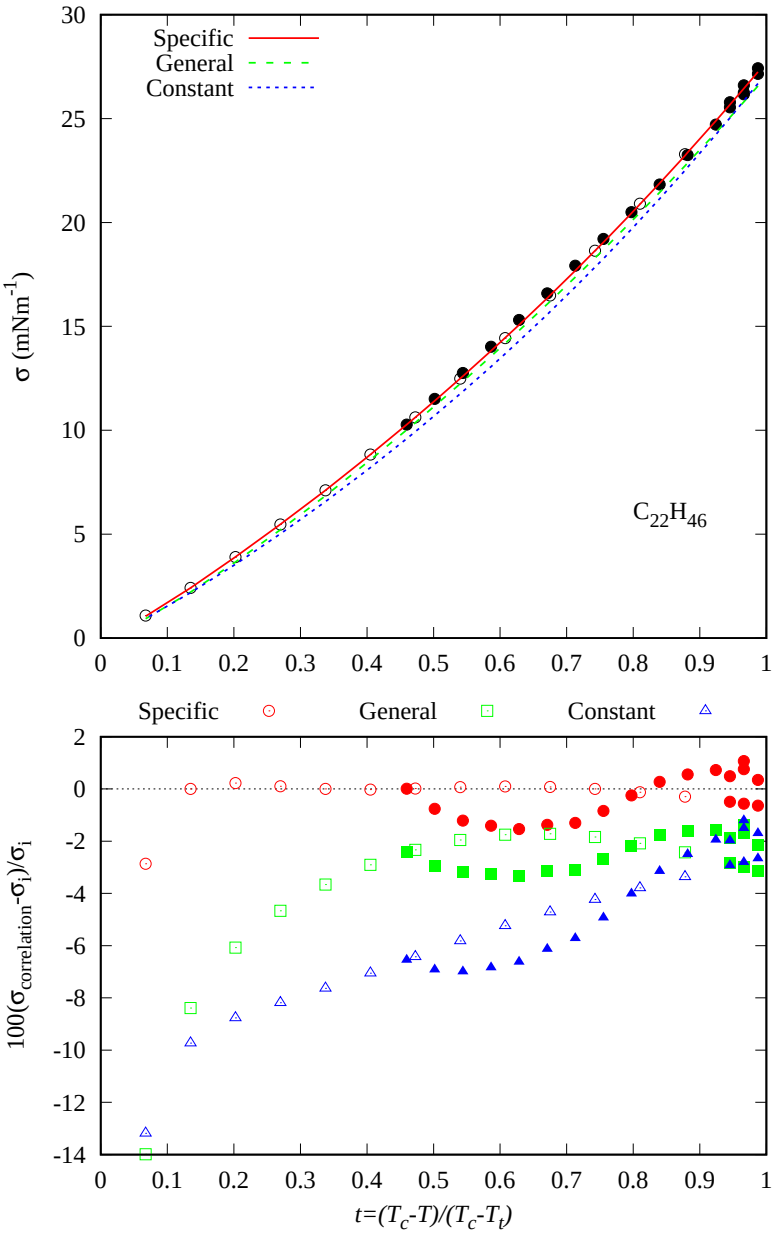

Figure 22. Surface tension data for *n*-docosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

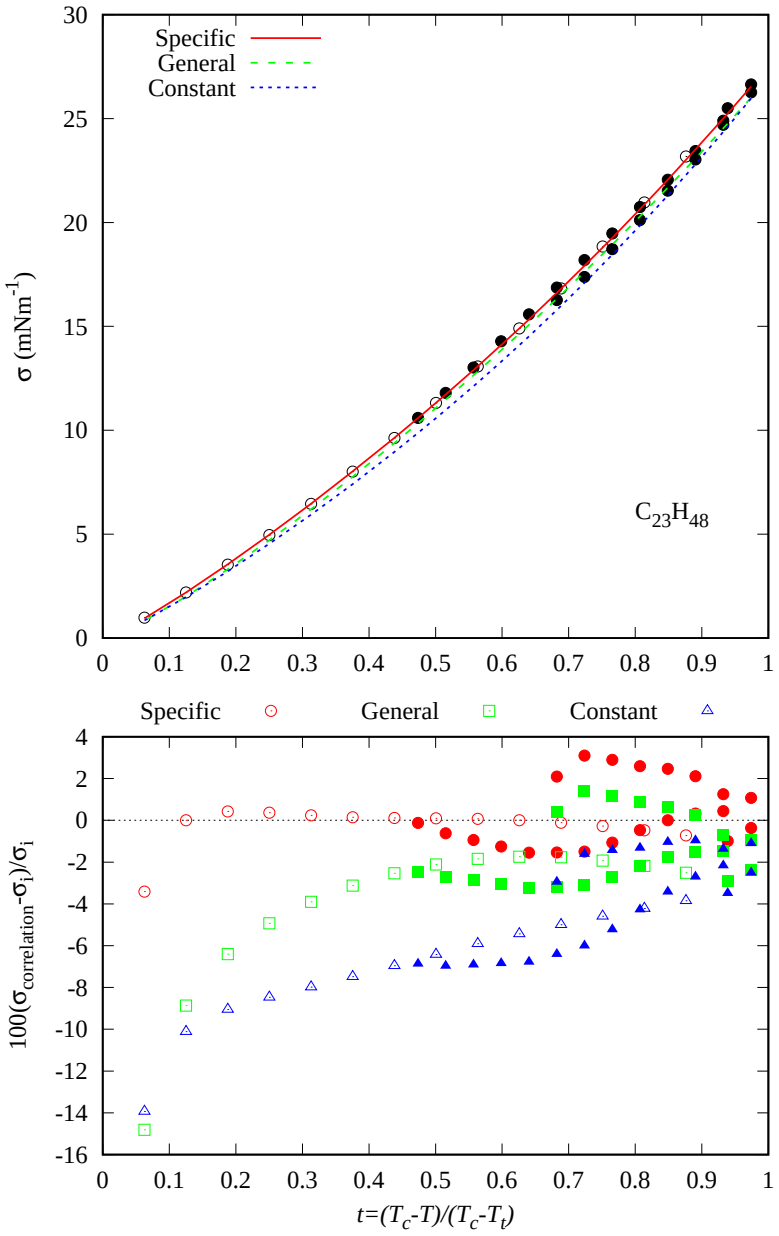

Figure 23. Surface tension data for *n*-tricosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

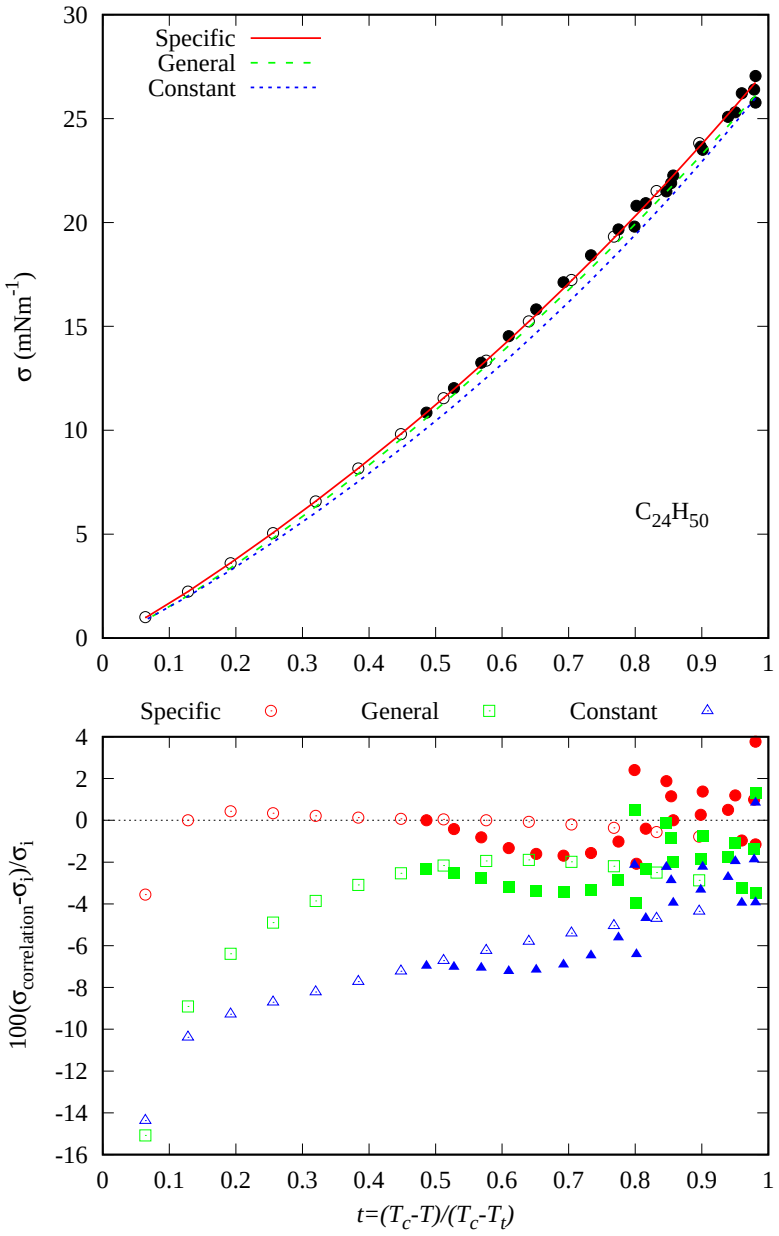

Figure 24. Surface tension data for *n*-tetracosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

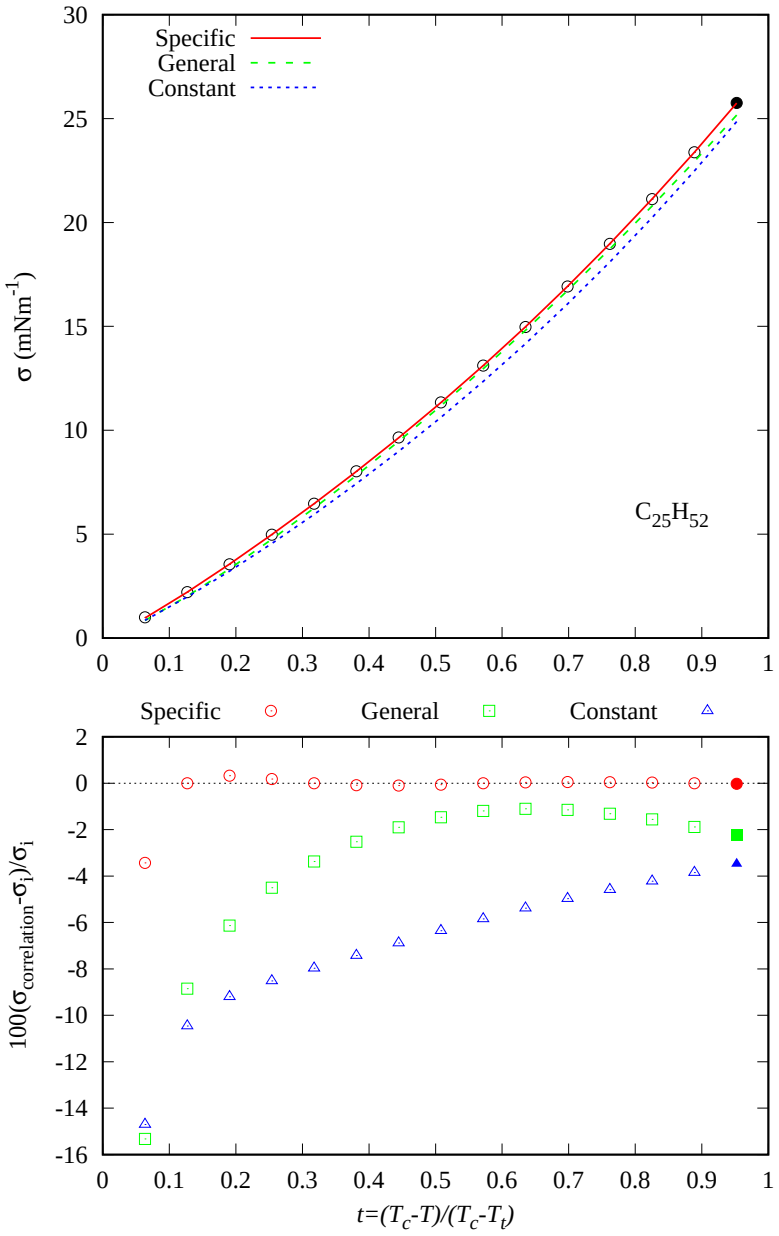

Figure 25. Surface tension data for *n*-pentacosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

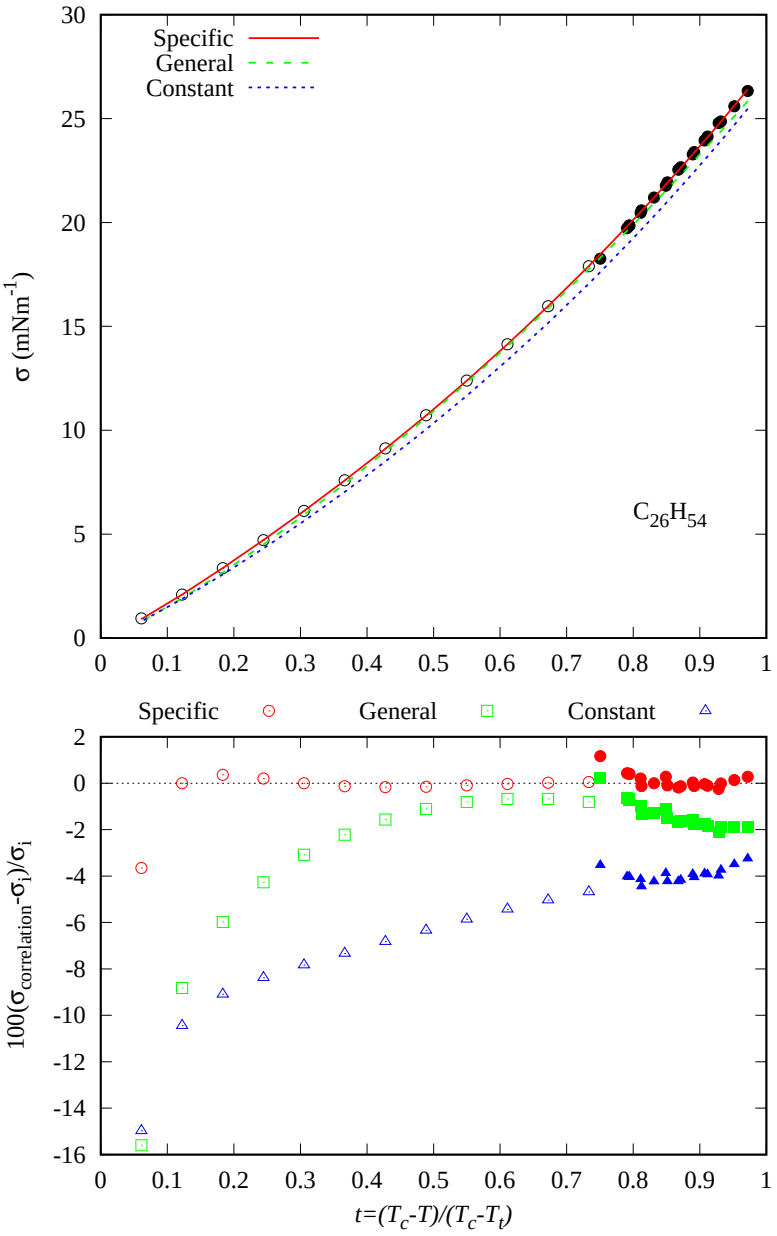

Figure 26. Surface tension data for *n*-hexacosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

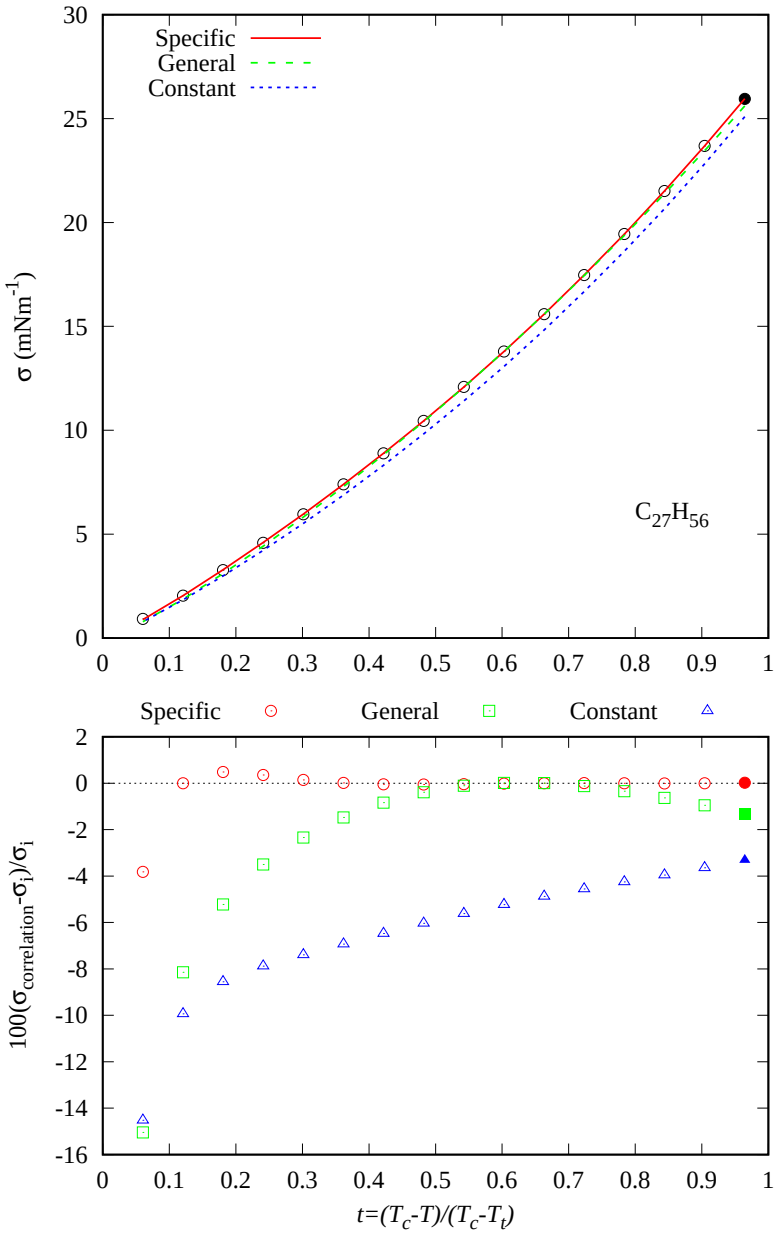

Figure 27. Surface tension data for *n*-heptacosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

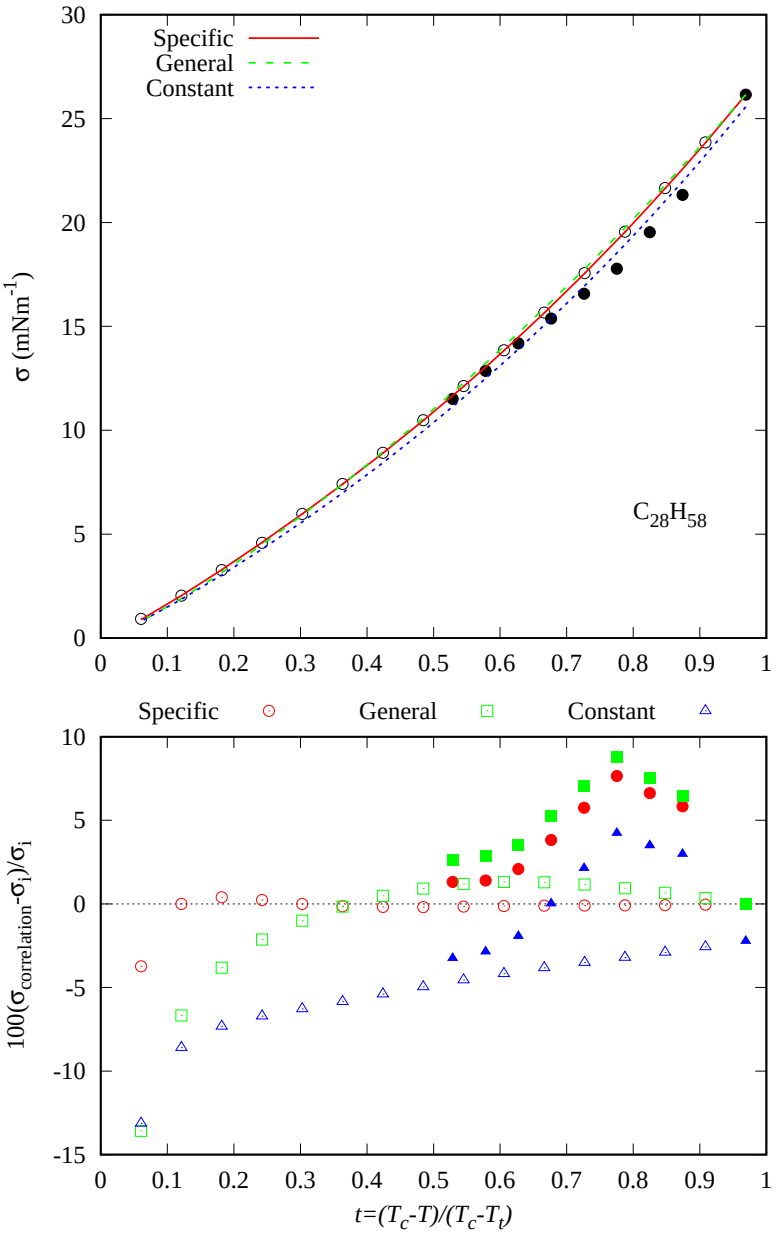

Figure 28. Surface tension data for *n*-octacosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

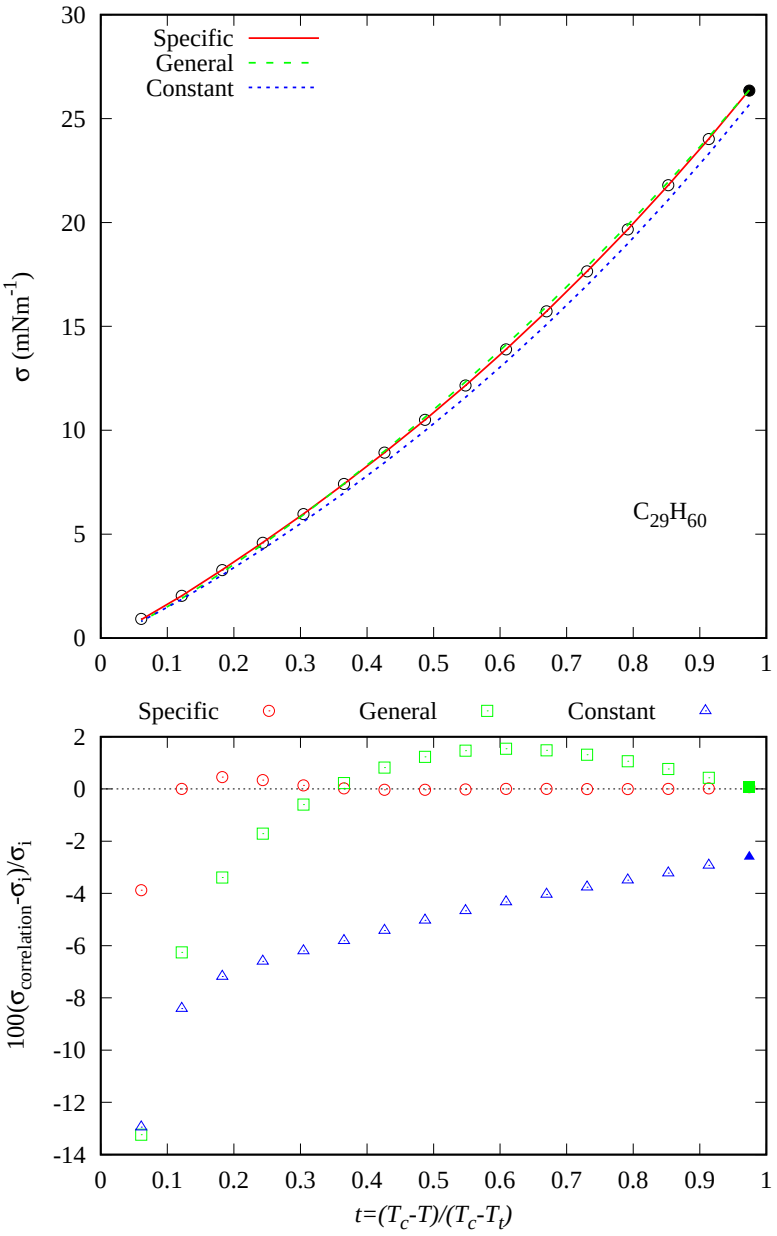

Figure 29. Surface tension data for *n*-nonacosane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

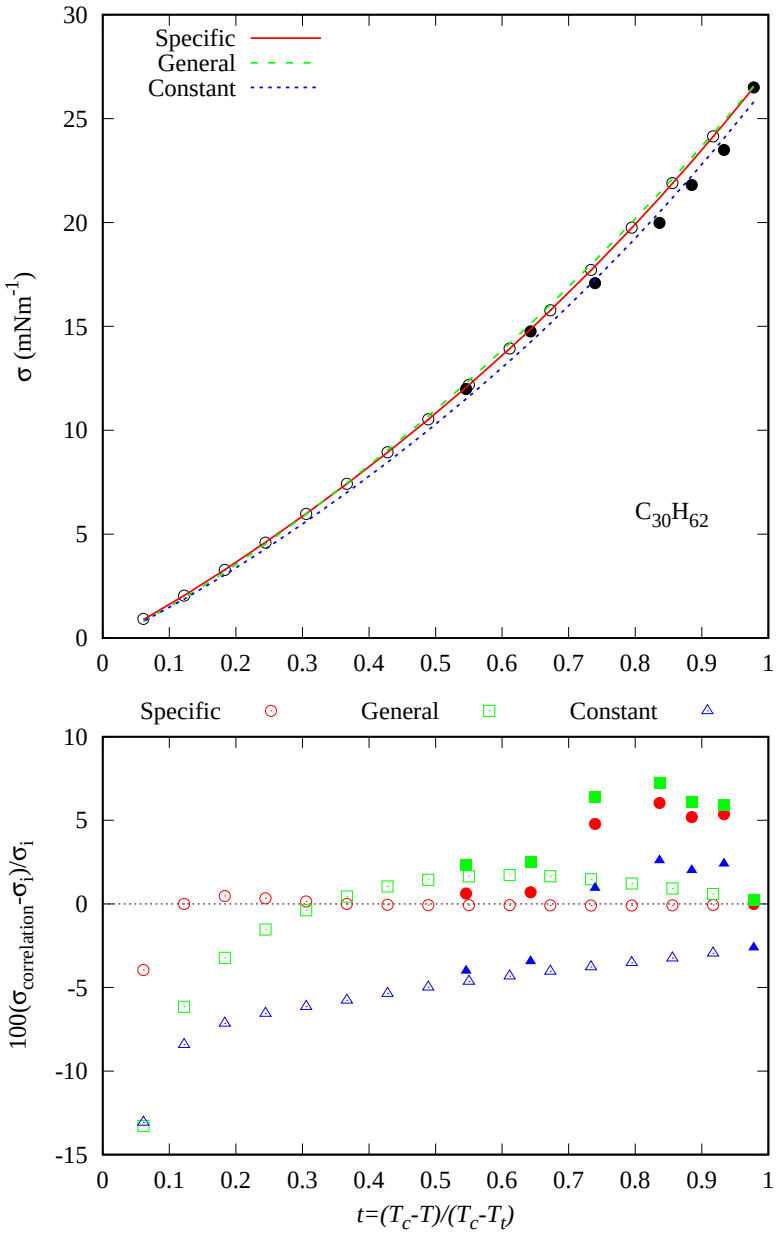

Figure 30. Surface tension data for *n*-triacontane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

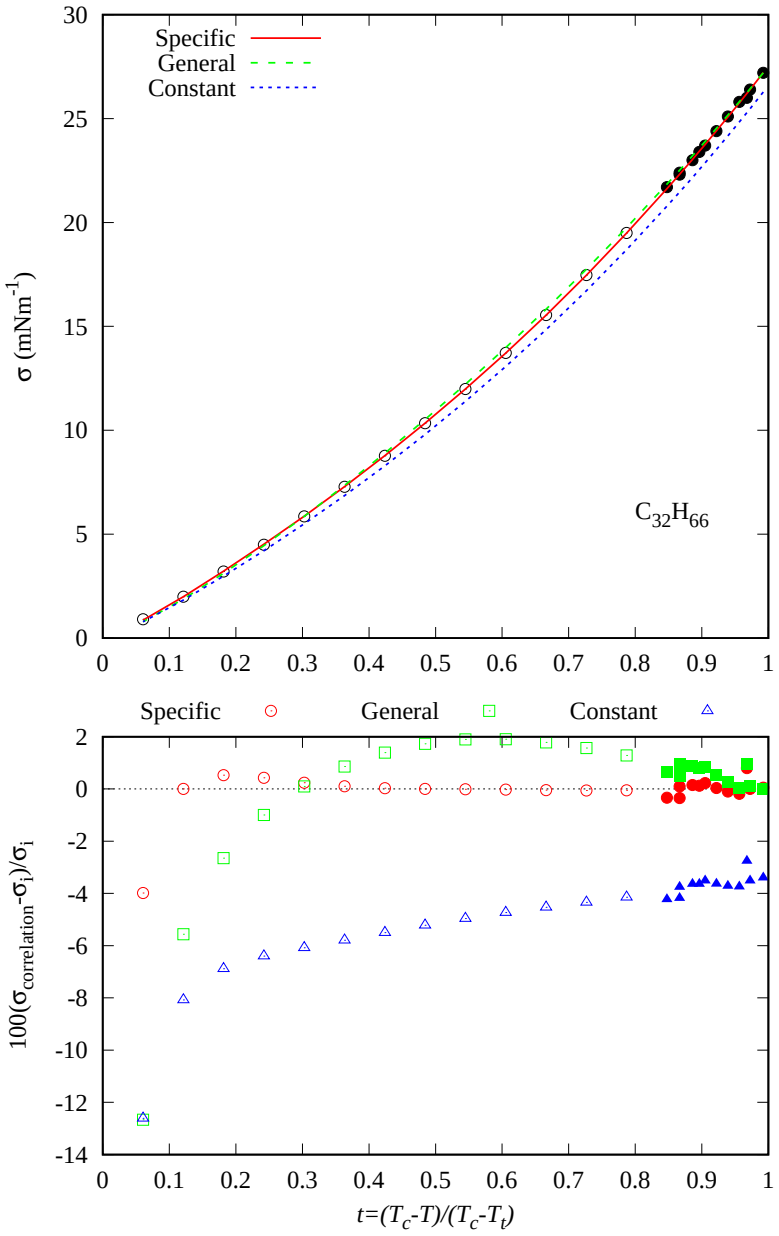

Figure 31. Surface tension data for *n*-dotriacontane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

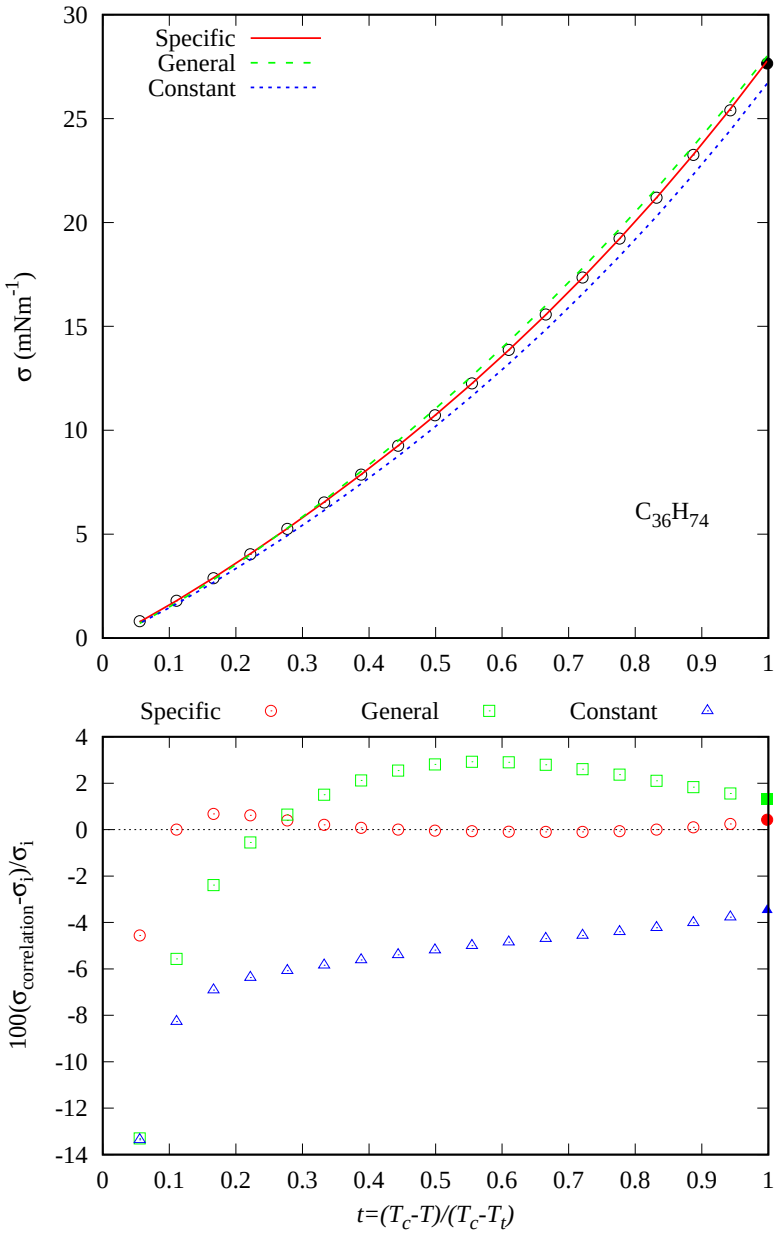

Figure 32. Surface tension data for *n*-hexatriacontane and percentage deviations from the correlations considered here (lines). The open symbols are the data from Sugden's correlation included in the DIPPR database. Closed symbols represent the fitting set data.

Table 1. Statistical figures of the global correlation when $m_0 = 4.99955$, $m_2 = -3.45186$ and $m_1 = 0.625431x^{-0.452929} + 3.52179x^{0.405698}$ (all in 10^{-17} mol$^{2/3}$ units), with x being the acentric factor. CN is the carbon number, N the number of data, MAPD the mean absolute percentage deviation, MD the mean deviation, PD_m the maximum absolute percentage deviation, and t_{PDm} is the reduced temperature of the maximum percentage deviation. The subscript fit is added for those figures calculated with the fitting set.

CN	N/N_{fit}	MAPD/MAPD$_{fit}$ (%)	MD/MD$_{fit}$ (%)	PD$_m$ /PD$_{m\ fit}$ (%)	$t_{PDm}/t_{PDm_{fit}}$
1	127/126	2.39/2.37	0.09/ 0.13	14.17/14.17	0.11/ 0.11
2	163/160	6.33/6.17	-5.97/-5.91	20.64/11.87	0.01/ 0.04
3	193/191	2.47/2.28	-1.64/-1.44	26.98/24.35	0.01/ 0.06
4	126/118	6.39/4.17	-0.45/-3.13	64.95/11.78	0.01/ 1.00
5	149/143	3.36/2.22	0.44/-0.82	51.58/11.53	0.01/ 0.02
6	270/269	2.73/2.70	-1.18/-1.23	13.47/13.47	0.07/ 0.07
7	363/357	1.88/1.74	0.66/ 0.50	14.95/14.95	0.05/ 0.05
8	196/194	1.96/1.64	-0.54/-0.89	36.19/6.09	0.01/ 0.19
9	78	0.88	0.27	4.97	0.54
10	149	2.02	1.44	10.54	0.12
11	60	2.44	2.42	14.18	0.30
12	100	3.06	3.04	8.12	0.91
13	48	2.48	2.48	5.95	0.69
14	49	1.47	1.34	5.37	0.72
15	40	2.60	2.60	6.36	0.74
16	127/117	1.97/1.94	0.60/ 0.65	10.45/10.45	0.40/ 0.40
17	44/ 34	1.45/1.13	0.55/ 0.52	6.84/3.64	0.07/ 0.78
18	39/ 29	1.51/1.19	-0.11/ 0.02	8.85/2.99	0.07/ 0.79
19	23/ 12	2.08/1.51	-0.02/ 0.27	10.01/4.65	0.07/ 0.34
20	38/ 25	1.94/1.90	-1.23/-1.05	12.37/12.37	0.33/ 0.33
21	28/ 14	2.15/1.35	-2.15/-1.35	13.44/2.53	0.07/ 0.92
22	32/ 19	1.71/1.33	-1.68/-1.33	12.41/2.90	0.07/ 0.99
23	36/ 22	1.74/1.35	-1.02/-0.22	13.32/2.98	0.06/ 0.72
24	36/ 22	1.82/1.38	-1.60/-1.04	13.61/3.36	0.06/ 0.98
25	15/ 1	2.30/1.94	-1.90/-1.94	13.86/1.94	0.06/ 0.95
26	31/ 19	1.64/0.93	-1.10/-0.65	14.18/1.75	0.06/ 0.97
27	16/ 1	2.30/1.30	-0.97/-1.30	13.67/1.30	0.06/ 0.96
28	24/ 9	4.33/6.43	2.82/ 6.43	12.08/10.26	0.06/ 0.78
29	16/ 1	2.89/0.18	0.74/ 0.18	11.80/0.18	0.06/ 0.97
30	22/ 7	3.97/5.51	2.44/ 5.51	11.81/8.24	0.06/ 0.84
32	25/ 12	2.29/0.94	1.07/ 0.93	11.23/1.63	0.06/ 0.87
36	18/ 1	3.74/1.15	1.97/ 1.15	11.96/1.15	0.06/ 1.00
Overall	2681/3427			64.95/24.35	
	N_{fluid}	OMAPD/ OMAPD$_{fit}$	OMD/ OMD$_{fit}$		
	32	2.57/2.18	0.11/0.24		

Table 2. Statistical figures of the global correlation when $m_0 = 4.91156$, $m_2 = -2.6442$ and $m_1 = 1.09159x^{-0.53364} + 2.68771x^{0.401163}$ (all in 10^{-17} mol$^{2/3}$ units), with x being the critical volume. CN is the carbon number, N the number of data, MAPD the mean absolute percentage deviation, MD the mean deviation, PD_m the maximum absolute percentage deviation, and t_{PDm} is the reduced temperature of the maximum percentage deviation. The subscript fit is added for those figures calculated with the fitting set.

CN	N/N_{fit}	MAPD/MAPD$_{fit}$ (%)	MD/MD$_{fit}$ (%)	PD$_m$ /PD$_{m\ fit}$ (%)	$t_{PDm}/t_{PDm_{fit}}$
1	127/126	5.43/5.40	-5.43/-5.40	18.65/18.65	0.11/ 0.11
2	163/160	3.38/3.16	0.83/ 1.02	20.71/11.38	0.01/ 0.04
3	193/191	2.00/1.81	0.46/ 0.68	27.36/24.37	0.01/ 0.06
4	126/118	4.20/1.92	1.92/-0.51	63.50/9.09	0.01/ 0.03
5	149/143	2.42/1.30	1.96/ 0.83	49.93/10.17	0.01/ 0.02
6	270/269	1.52/1.49	-0.28/-0.32	11.46/11.46	0.07/ 0.07
7	363/357	1.18/1.05	0.80/ 0.67	12.63/12.63	0.05/ 0.05
8	196/194	1.33/1.02	-0.47/-0.80	34.16/3.56	0.01/ 0.77
9	78	0.49	0.34	3.13	0.80
10	149	1.35	0.72	6.97	0.12
11	60	1.42	1.42	10.04	0.30
12	100	1.94	1.91	7.84	0.91
13	48	1.32	1.32	3.42	0.69
14	49	0.81	0.46	4.67	0.40
15	40	1.54	1.54	3.95	0.74
16	127/117	1.73/1.61	-0.51/-0.28	10.01/6.28	0.08/ 0.46
17	44/ 34	1.32/0.85	-1.12/-0.60	9.90/1.68	0.07/ 0.78
18	39/ 29	1.77/1.02	-1.66/-0.89	11.86/2.48	0.07/ 0.99
19	23/ 12	2.56/1.48	-2.30/-0.98	12.93/8.45	0.07/ 0.34
20	38/ 25	2.92/2.03	-2.73/-1.75	15.85/15.85	0.33/ 0.33
21	28/ 14	4.56/3.40	-4.56/-3.40	16.20/4.75	0.07/ 0.49
22	32/ 19	3.71/2.78	-3.71/-2.78	15.20/4.14	0.07/ 0.54
23	36/ 22	3.24/2.06	-3.06/-1.78	15.99/3.91	0.06/ 0.64
24	36/ 22	3.43/2.36	-3.32/-2.18	16.23/4.11	0.06/ 0.80
25	15/ 1	4.35/1.93	-4.35/-1.93	16.45/1.93	0.06/ 0.95
26	31/ 19	2.58/1.24	-2.58/-1.24	16.69/1.76	0.06/ 0.93
27	16/ 1	3.21/0.91	-3.21/-0.91	16.16/0.91	0.06/ 0.96
28	24/ 9	3.49/4.81	0.64/ 4.81	14.65/8.82	0.06/ 0.78
29	16/ 1	2.49/0.68	-1.47/ 0.68	14.32/0.68	0.06/ 0.97
30	22/ 7	3.35/4.66	0.61/ 4.66	14.31/7.60	0.06/ 0.84
32	25/ 12	2.17/1.40	0.06/ 1.40	13.62/2.00	0.06/ 0.97
36	18/ 1	3.32/2.80	0.54/ 2.80	14.15/2.80	0.06/ 1.00
Overall	2681/2427			63.50/24.37	
	N_{fluid}	OMAPD/ OMAPD$_{fit}$	OMD/ OMD$_{fit}$		
	32	2.52/1.94	-0.79/-0.02		

Table 3. Statistical figures of the global correlation when $m_0 = 5.37325$, $m_2 = 2.05972$ and $m_1 = 0.662073x^{-0.595946} + 4.84453x^{0.542305}$ (all in 10^{-17} mol$^{2/3}$ units), with x being the liquid molar volume at 298.15 K and 101325 Pa. CN is the carbon number, N the number of data, MAPD the mean absolute percentage deviation, MD the mean deviation, PD_m the maximum absolute percentage deviation, and t_{PDm} is the reduced temperature of the maximum percentage deviation. The subscript fit is added for those figures calculated with the fitting set.

CN	N/N_{fit}	MAPD/MAPD$_{fit}$ (%)	MD/MD$_{fit}$ (%)	PD$_m$ /PD$_{m\ fit}$ (%)	$t_{PDm}/t_{PDm_{fit}}$
1	127/126	3.35/3.33	-1.43/-1.40	16.82/16.82	0.11/ 0.11
2	163/160	3.44/3.22	-2.54/-2.44	19.07/11.63	0.01/ 0.15
3	193/191	2.08/1.91	-0.47/-0.28	25.46/23.76	0.01/ 0.06
4	126/118	4.79/2.29	1.76/-0.94	68.36/11.25	0.01/ 0.03
5	149/143	2.97/1.72	1.77/ 0.47	54.88/12.73	0.01/ 0.02
6	270/269	1.97/1.93	-0.54/-0.59	12.54/12.32	0.01/ 0.04
7	363/357	1.43/1.26	0.59/ 0.41	14.97/14.01	0.01/ 0.05
8	196/194	1.51/1.16	-0.52/-0.89	38.48/3.59	0.01/ 0.21
9	78	0.65	0.46	3.40	0.80
10	149	1.29	0.69	6.70	0.12
11	60	1.35	1.33	8.28	0.30
12	100	2.01	1.94	8.54	0.91
13	48	1.41	1.41	2.47	0.69
14	49	0.99	0.66	6.51	0.40
15	40	1.77	1.73	3.08	0.74
16	127/117	1.53/1.28	-0.50/-0.17	9.79/4.87	0.08/ 0.81
17	44/ 34	1.65/0.86	-1.58/-0.77	9.60/2.53	0.07/ 0.60
18	39/ 29	2.05/0.93	-2.03/-0.89	11.60/1.80	0.07/ 0.99
19	23/ 12	3.20/1.41	-3.10/-1.22	12.57/10.33	0.07/ 0.34
20	38/ 25	3.20/1.80	-3.12/-1.68	17.58/17.58	0.33/ 0.33
21	28/ 14	5.58/4.35	-5.58/-4.35	15.84/6.64	0.07/ 0.49
22	32/ 19	4.55/3.34	-4.55/-3.34	14.88/5.91	0.07/ 0.54
23	36/ 22	4.00/2.54	-3.99/-2.51	15.58/5.53	0.06/ 0.52
24	36/ 22	4.25/2.94	-4.12/-2.74	15.85/5.39	0.06/ 0.61
25	15/ 1	5.41/1.59	-5.41/-1.59	16.05/1.59	0.06/ 0.95
26	31/ 19	3.21/1.44	-3.21/-1.44	16.23/1.87	0.06/ 0.81
27	16/ 1	4.23/0.48	-4.23/-0.48	15.68/0.48	0.06/ 0.96
28	24/ 9	3.48/3.92	-0.39/ 3.92	14.16/8.05	0.06/ 0.78
29	16/ 1	2.90/1.20	-2.47/ 1.20	13.85/1.20	0.06/ 0.97
30	22/ 7	3.32/4.17	-0.28/ 4.17	13.83/7.25	0.06/ 0.84
32	25/ 12	2.24/1.59	-0.48/ 1.59	13.13/2.50	0.06/ 0.97
36	18/ 1	3.01/3.68	-0.23/ 3.68	13.50/3.68	0.06/ 1.00
Overall	2681/2427			68.36/23.76	
	N_{fluid}	OMAPD/ OMAPD$_{fit}$	OMD/ OMD$_{fit}$		
	32	2.78/1.99	-1.20/-0.13		