

Tridecafluorheptansäure C₇H₁F₁₃O₂

Gemessen im negativen Modus:

[M-H]⁻ [C₇F₁₃O₂]⁻ exakte Masse m/z= 362.9696

10ppm bedeutet bei m/z 400 $400 \cdot (10/10^6) = 0.0040$ m/z

5ppm bedeutet bei m/z 400 $400 \cdot (5/10^6) = 0.0020$ m/z

1ppm bedeutet bei m/z 400 $400 \cdot (1/10^6) = 0.0004$ m/z

Massengenauigkeit 10ppm -> 30 Vorschläge

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
362.9700	1	C4HF10N2O6	362.9680	-5.3	8.7	1	44.78	0.5	even	ok
	2	C3H3F8N2O9	362.9716	4.6	11.2	2	51.76	-0.5	even	ok
	3	CF5N8O9	362.9714	3.9	11.3	3	60.80	3.5	even	ok
	4	C6H2F11O5	362.9732	8.9	13.9	4	12.74	0.5	even	ok
	5	C3H3F4N4O12	362.9689	-2.9	15.3	5	70.20	2.5	even	ok
	6	CFN10O12	362.9687	-3.6	15.3	6	60.66	6.5	even	ok
	7	CH2F7N4O10	362.9665	-9.7	15.5	7	9.35	-0.5	even	ok
	8	C7F13O2	362.9696	-1.0	17.9	8	96.23	1.5	even	ok
	9	C2H5F2N4O15	362.9725	7.0	18.4	9	22.81	1.5	even	ok
	10	C6H2F7N2O8	362.9705	1.4	20.1	10	84.76	3.5	even	ok
	11	C5H6F3O15	362.9664	-9.8	20.4	11	8.12	1.5	even	ok
	12	C4H8FO18	362.9700	0.1	22.1	12	100.00	0.5	even	ok
	13	C7F9N2O5	362.9669	-8.5	23.6	13	12.31	4.5	even	ok
	14	C5H4FN4O14	362.9714	3.8	24.3	14	47.47	5.5	even	ok
	15	C6H2F3N4O11	362.9678	-6.1	26.4	15	25.08	6.5	even	ok
	16	C7H7O17	362.9689	-3.0	30.5	16	49.00	4.5	even	ok
	17	C9HF10O4	362.9721	5.8	31.3	17	24.25	4.5	even	ok
	18	C6FN8O10	362.9727	7.5	33.1	18	13.65	10.5	even	ok
	19	C8H3F4N2O10	362.9729	8.2	33.1	19	10.89	6.5	even	ok
	20	C9HF6N2O7	362.9693	-1.7	37.1	20	53.57	7.5	even	ok
	21	C8H3N4O13	362.9702	0.7	39.3	21	60.43	9.5	even	ok
	22	C9HF2N4O10	362.9666	-9.2	43.1	22	5.69	10.5	even	ok
	23	C12F9O3	362.9709	2.6	49.6	23	31.57	8.5	even	ok
	24	C11H2F3N2O9	362.9718	5.0	50.6	24	17.49	10.5	even	ok
	25	C12F5N2O6	362.9682	-4.9	55.2	25	15.75	11.5	even	ok
	26	C14HF6O5	362.9734	9.4	63.1	26	2.86	11.5	even	ok
	27	C14HF2N2O8	362.9706	1.9	68.8	27	19.23	14.5	even	ok
	28	C17F5O4	362.9722	6.2	81.6	28	4.13	15.5	even	ok
	29	C17FN2O7	362.9695	-1.3	87.2	29	10.25	18.5	even	ok
	30	C22FO5	362.9735	9.8	113.9	30	0.27	22.5	even	ok

Massengenauigkeit 5ppm -> 16 Vorschläge

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
362.9700	1	C3H3F8N2O9	362.9716	4.6	11.2	1	51.76	-0.5	even	ok
	2	CF5N8O9	362.9714	3.9	11.3	2	60.80	3.5	even	ok
	3	C3H3F4N4O12	362.9689	-2.9	15.3	3	70.20	2.5	even	ok
	4	CFN10O12	362.9687	-3.6	15.3	4	60.66	6.5	even	ok
	5	C7F13O2	362.9696	-1.0	17.9	5	96.23	1.5	even	ok
	6	C6H2F7N2O8	362.9705	1.4	20.1	6	84.76	3.5	even	ok
	7	C4H8FO18	362.9700	0.1	22.1	7	100.00	0.5	even	ok
	8	C5H4FN4O14	362.9714	3.8	24.3	8	47.47	5.5	even	ok
	9	C7H7O17	362.9689	-3.0	30.5	9	49.00	4.5	even	ok
	10	C9HF6N2O7	362.9693	-1.7	37.1	10	53.57	7.5	even	ok
	11	C8H3N4O13	362.9702	0.7	39.3	11	60.43	9.5	even	ok
	12	C12F9O3	362.9709	2.6	49.6	12	31.57	8.5	even	ok
	13	C11H2F3N2O9	362.9718	5.0	50.6	13	17.49	10.5	even	ok
	14	C12F5N2O6	362.9682	-4.9	55.2	14	15.75	11.5	even	ok
	15	C14HF2N2O8	362.9706	1.9	68.8	15	19.23	14.5	even	ok
	16	C17FN2O7	362.9695	-1.3	87.2	16	10.25	18.5	even	ok

Massengenauigkeit 1ppm -> 3 Vorschläg

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
362.9700	1	C7F13O2	362.9696	-1.0	17.9	1	96.23	1.5	even	ok
	2	C4H8FO18	362.9700	0.1	22.1	2	100.00	0.5	even	ok
	3	C8H3N4O13	362.9702	0.7	39.3	3	60.43	9.5	even	ok

Durch Vergleich der Isotopenmuster ist die eindeutige Zuordnung der gesuchten Verbindung möglich! (bei einer Massengenauigkeit von 1ppm)

