

Automated Solvent Extraction of NIST SRM 1941b, Organics in Marine Sediment, on Rxi®-PAH

Peaks	Peaks
1. Naphthalene-d8	24. 5-Methylchrysene
2. Naphthalene	25. Benzo[b]fluoranthene
3. 2-Methylnaphthalene	26. Benzo[k]fluoranthene
4. Biphenyl	27. Benzo[j]fluoranthene
5. Acenaphthylene	28. Benzo[a]fluoranthene
6. Acenaphthene-d10	29. Benzo[e]pyrene
7. Acenaphthene	30. Benzo[a]pyrene
8. Fluorene	31. Perylene-d12
9. Dibenzothiophene	32. Perylene
10. Phenanthrene-d10	33. Dibenzo[a,j]anthracene
11. Phenanthrene	34. Dibenzo[a,c]anthracene
12. Anthracene	35. Indeno[1,2,3-cd]pyrene
13. 4H-Cyclopenta[def]phenanthrene	36. Dibenzo[a,h]anthracene
14. Fluoranthene	37. Benzo[b]chrysene
15. Pyrene	38. Picene
16. Benzo[c]fluorene	39. Benzo[ghi]perylene
17. Benzo[ghi]fluoranthene	40. Anthanthrene
18. Benzo[c]phenanthrene	41. Dibenzo[b,k]fluoranthene
19. Benz[a]anthracene	42. Dibenzo[a,e]pyrene
20. Chrysene-d12	43. Coronene-d12
21. Cyclopenta[cd]pyrene	44. Coronene
22. Triphenylene	45. Dibenzo[a,i]pyrene
23. Chrysene	46. Dibenzo[a,h]pyrene

Scan Program:	Group	Start Time (min)	Ion(s) (m/z)	Dwell (ms)
	1	3.09	102.1, 108.1, 128.1, 136.2	40
	2	5.69	115.1, 142.1	40
	3	6.23	76.1, 141.1, 154.1, 156.2	40
	4	6.95	75.6, 76.1, 91.1, 152.1, 153.1, 155.1, 162.2, 170.2	20
	5	7.93	82.4, 165.1	40
	6	9.19	139.1, 152.1, 160.2, 178.1, 184.1, 188.2	40
	7	11.78	94.6, 165.1, 190.1, 192.1	40
	8	14.19	101.1, 202.1	40
	9	16.60	101.1, 202.1	40
	10	18.49	92.1, 184.1	40
	11	19.58	108, 216	40
	12	22.3	196.1, 212.2	40
	13	24.92	113.1, 226.1, 228.1	40
	14	26.27	113.1, 114.0, 120.1, 226.1, 228.1, 240.1	40
	15	28.75	154.1, 252.1	35
	16	30.62	119.8, 242.2	40
	17	35.29	126.1, 252.1	40
	18	38.56	125.1, 252.1	40
	19	39.23	126.1, 252.1	40
	20	40.71	125.1, 126.1, 132.1, 252.1, 264.1	40
	21	42.91	125, 132.2, 252.1, 264.1	40
	22	44.35	252.1, 268.1	40
	23	48.41	139.1, 139.5, 278.1, 279.1	40
	24	52.13	139.1, 139.5, 278.1, 279.1	40
	25	53.70	138.1, 139.1, 278.1	40
	26	54.97	138.1, 276.1	40
	27	55.92	138.1, 276.1	40
	28	57.04	132.6, 267.1	40
	29	59.69	151.0, 302.1	40
	30	63.27	150, 151, 156.1, 300.1, 302.1, 312.1	40
	31	64.78	151.0, 302.1	40

Column Rxi®-PAH, 60 m, 0.25 mm ID, 0.10 µm (cat.# 49317)
Sample SV internal standard mix (cat.# 31206)
 Coronene-d12 (CIL DLM-2715)
 Benzo[a]pyrene-d12 (CIL DLM-258-0)
 Aromatics in toluene (NIST SRM-2260a)
 PAH native stock solution (Wellington PAH-STK-B)
 Dichloromethane

Diluent:
Injection
 Inj. Vol.: 1 µL split (split ratio 10:1)
 Liner: Premium 4 mm Precision liner w/wool (cat.# 23305.1)
 Inj. Temp.: 275 °C
 Split Vent Flow Rate: 19.5 mL/min

Oven
 Oven Temp.: 110 °C (hold 1.6 min) to 210 °C at 24 °C/min to 295 °C at 1.9 °C/min to 350 °C at 3.7 °C/min (hold 6 min)

Carrier Gas
 Flow Rate: He, constant flow
 1.95 mL/min

Detector MS
 Mode: SIM
 Transfer Line Temp.: 330 °C
 Analyzer Type: Quadrupole
 Source Type: Extractor
 Extractor Lens: 9 mm ID
 Source Temp.: 350 °C
 Quad Temp.: 200 °C
 Solvent Delay Time: 3 min
 Tune Type: DFTPP
 Ionization Mode: EI
Instrument Agilent 7890B GC & 5977A MSD
Notes Performs the separation of two critical sets of isobars:
 1. Cyclopenta[c,d]pyrene, triphenylene, and chrysene
 2. Benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene

