

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120621\
 Data File : VY006969.D
 Acq On : 06 Dec 2021 18:25
 Operator : SY/MD
 Sample : M4887-15
 Misc : 4.37g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EX8C9

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
 Title : VOC Analysis

Signal : TIC: VY006969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.247	65	70	79	rVB	33472	58973	3.91%	1.938%
2	2.765	149	155	167	rVB2	19633	47804	3.17%	1.571%
3	3.497	273	275	278	rBV2	255	258	0.02%	0.008%
4	3.680	304	305	306	rVB	275	101	0.01%	0.003%
5	3.704	306	309	311	rBV2	300	303	0.02%	0.010%
6	3.777	320	321	323	rBV2	258	186	0.01%	0.006%
7	3.845	323	332	348	rBV3	28898	94931	6.30%	3.120%
8	4.009	358	359	361	rBV	229	153	0.01%	0.005%
9	4.113	374	376	377	rBV	144	109	0.01%	0.004%
10	4.131	377	379	381	rVV2	206	187	0.01%	0.006%
11	4.186	381	388	399	rVB3	2004	5767	0.38%	0.190%
12	4.265	399	401	403	rBV	205	161	0.01%	0.005%
13	4.283	403	404	407	rVB	241	232	0.02%	0.008%
14	4.363	415	417	419	rBV	396	403	0.03%	0.013%
15	4.393	419	422	423	rVV2	456	364	0.02%	0.012%
16	4.588	450	454	456	rBV2	155	256	0.02%	0.008%
17	4.710	463	474	484	rBV3	10962	34354	2.28%	1.129%
18	4.850	493	497	498	rBV2	215	304	0.02%	0.010%
19	5.107	536	539	540	rBV	259	255	0.02%	0.008%
20	5.186	549	552	554	rBV2	216	357	0.02%	0.012%
21	5.228	557	559	560	rBV	121	126	0.01%	0.004%
22	5.424	585	591	592	rBV	227	383	0.03%	0.013%
23	5.497	600	603	606	rBV	267	281	0.02%	0.009%
24	5.747	634	644	652	rBV5	1611	5213	0.35%	0.171%
25	5.826	655	657	660	rBV3	238	312	0.02%	0.010%
26	5.972	679	681	684	rVB2	202	224	0.01%	0.007%
27	6.003	684	686	690	rVB2	208	188	0.01%	0.006%
28	6.058	693	695	698	rBV2	222	223	0.01%	0.007%
29	6.179	713	715	717	rBV	127	124	0.01%	0.004%
30	6.234	721	724	725	rBV	155	153	0.01%	0.005%
31	6.253	725	727	728	rBV	134	100	0.01%	0.003%
32	6.308	731	736	739	rBV2	264	622	0.04%	0.020%
33	6.387	747	749	752	rBV	308	300	0.02%	0.010%
34	6.417	752	754	757	rVB2	236	221	0.01%	0.007%
35	6.564	776	778	781	rVB	147	124	0.01%	0.004%
36	6.667	792	795	798	rBV3	285	332	0.02%	0.011%

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37	6.789	814	815	817	rBV	220	124	0.01%	0.004%
38	6.814	817	819	822	rVB	211	217	0.01%	0.007%
39	6.899	822	833	836	rBV3	2761	8026	0.53%	0.264%
40	7.478	918	928	940	rVB	43197	108136	7.17%	3.554%
41	7.563	940	942	943	rBV	233	190	0.01%	0.006%
42	7.606	948	949	952	rVB2	218	128	0.01%	0.004%
43	7.704	964	965	966	rBV2	270	180	0.01%	0.006%
44	7.874	991	993	995	rVB2	252	226	0.01%	0.007%
45	7.960	1005	1007	1008	rBV	176	110	0.01%	0.004%
46	8.106	1022	1031	1045	rBV4	91016	269909	17.90%	8.871%
47	8.234	1047	1052	1057	rVV3	2371	4818	0.32%	0.158%
48	8.344	1068	1070	1071	rBV	280	251	0.02%	0.008%
49	8.423	1082	1083	1085	rBV	331	303	0.02%	0.010%
50	8.569	1105	1107	1111	rVB2	371	353	0.02%	0.012%
51	8.685	1118	1126	1134	rBV	82404	163572	10.85%	5.376%
52	8.807	1144	1146	1148	rVB	184	104	0.01%	0.003%
53	8.935	1158	1167	1184	rBV	800268	1507476	100.00%	49.547%
54	9.057	1184	1187	1188	rBV2	307	282	0.02%	0.009%
55	9.118	1190	1197	1205	rVB2	50547	102344	6.79%	3.364%
56	9.447	1250	1251	1252	rBV	300	163	0.01%	0.005%
57	9.648	1283	1284	1286	rBV	181	147	0.01%	0.005%
58	9.783	1303	1306	1309	rBV2	173	193	0.01%	0.006%
59	9.886	1316	1323	1330	rBV2	15769	27855	1.85%	0.916%
60	9.935	1330	1331	1334	rVB2	363	249	0.02%	0.008%
61	9.971	1334	1337	1338	rBV	263	232	0.02%	0.008%
62	10.075	1347	1354	1357	rBV3	635	1412	0.09%	0.046%
63	10.179	1364	1371	1377	rBV	70144	120878	8.02%	3.973%
64	10.240	1377	1381	1386	rVB2	2947	4705	0.31%	0.155%
65	10.337	1394	1397	1399	rVB	270	276	0.02%	0.009%
66	10.435	1408	1413	1421	rVB	9174	15504	1.03%	0.510%
67	10.496	1421	1423	1425	rBV	337	300	0.02%	0.010%
68	10.575	1430	1436	1442	rVV	11333	18791	1.25%	0.618%
69	10.642	1442	1447	1452	rVV2	8666	14048	0.93%	0.462%
70	10.721	1453	1460	1464	rVV2	9312	16721	1.11%	0.550%
71	10.788	1464	1471	1482	rVV5	8397	23418	1.55%	0.770%
72	10.880	1484	1486	1487	rVB2	401	227	0.02%	0.007%
73	10.898	1487	1489	1491	rBV	262	275	0.02%	0.009%
74	10.941	1491	1496	1506	rVV	12100	20580	1.37%	0.676%
75	11.032	1509	1511	1514	rVB2	389	301	0.02%	0.010%
76	11.063	1514	1516	1520	rBV2	258	348	0.02%	0.011%

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77	11.319	1551	1558	1565	rVB2	10507	17136	1.14%	0.563%
78	11.483	1579	1585	1592	rBV	59434	97593	6.47%	3.208%
79	11.575	1598	1600	1601	rBV	253	231	0.02%	0.008%
80	11.727	1624	1625	1627	rBV	134	100	0.01%	0.003%
81	11.807	1636	1638	1639	rBV	267	136	0.01%	0.004%
82	11.910	1654	1655	1656	rBV	239	111	0.01%	0.004%
83	11.953	1661	1662	1664	rBV2	295	210	0.01%	0.007%
84	12.026	1671	1674	1679	rBV3	441	902	0.06%	0.030%
85	12.252	1709	1711	1714	rBV2	164	123	0.01%	0.004%
86	12.489	1740	1750	1756	rBV	47063	77926	5.17%	2.561%
87	12.556	1756	1761	1768	rVV2	31733	50627	3.36%	1.664%
88	12.623	1768	1772	1779	rVB4	740	1397	0.09%	0.046%
89	12.733	1788	1790	1794	rVB2	332	227	0.02%	0.007%
90	12.819	1800	1804	1810	rBV2	3549	5466	0.36%	0.180%
91	12.873	1812	1813	1815	rBV2	431	325	0.02%	0.011%
92	12.898	1815	1817	1820	rBV2	484	344	0.02%	0.011%
93	13.111	1850	1852	1854	rBV	381	290	0.02%	0.010%
94	13.178	1859	1863	1871	rVB3	4281	6773	0.45%	0.223%
95	13.276	1877	1879	1885	rVB4	1466	1955	0.13%	0.064%
96	13.422	1898	1903	1908	rVV	24564	35412	2.35%	1.164%
97	13.471	1908	1911	1921	rVB3	1669	3507	0.23%	0.115%
98	13.635	1935	1938	1942	rBV4	1253	2022	0.13%	0.066%
99	13.721	1946	1952	1958	rVB2	18519	28562	1.89%	0.939%
100	13.959	1985	1991	2000	rVB2	14060	23394	1.55%	0.769%

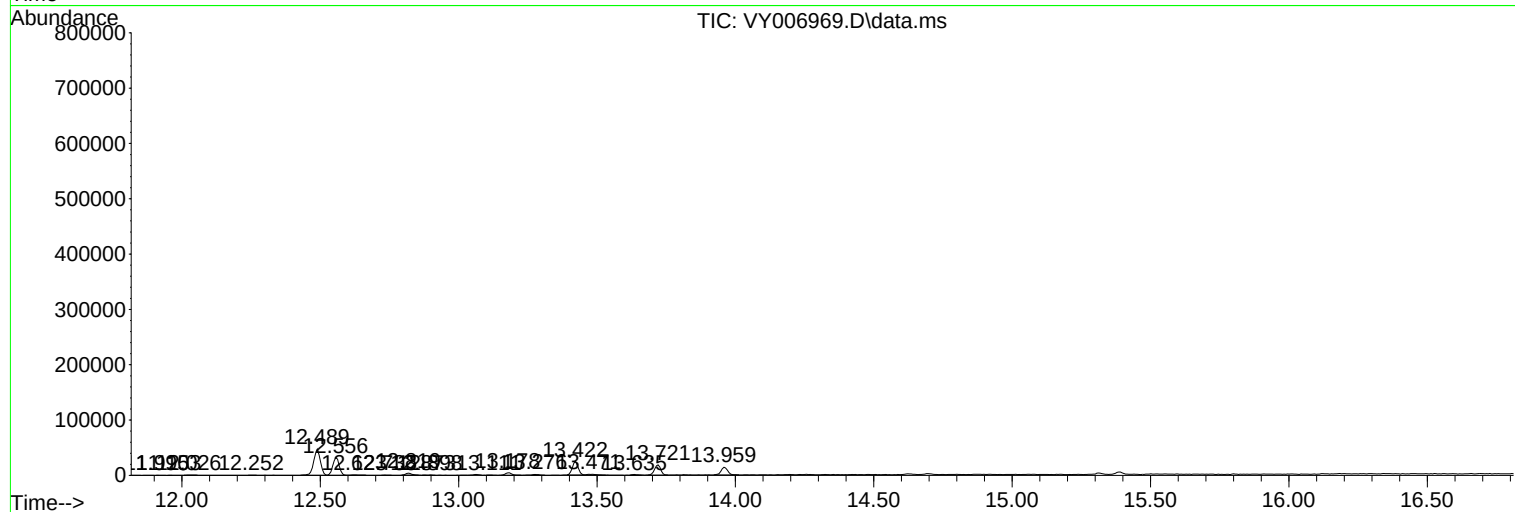
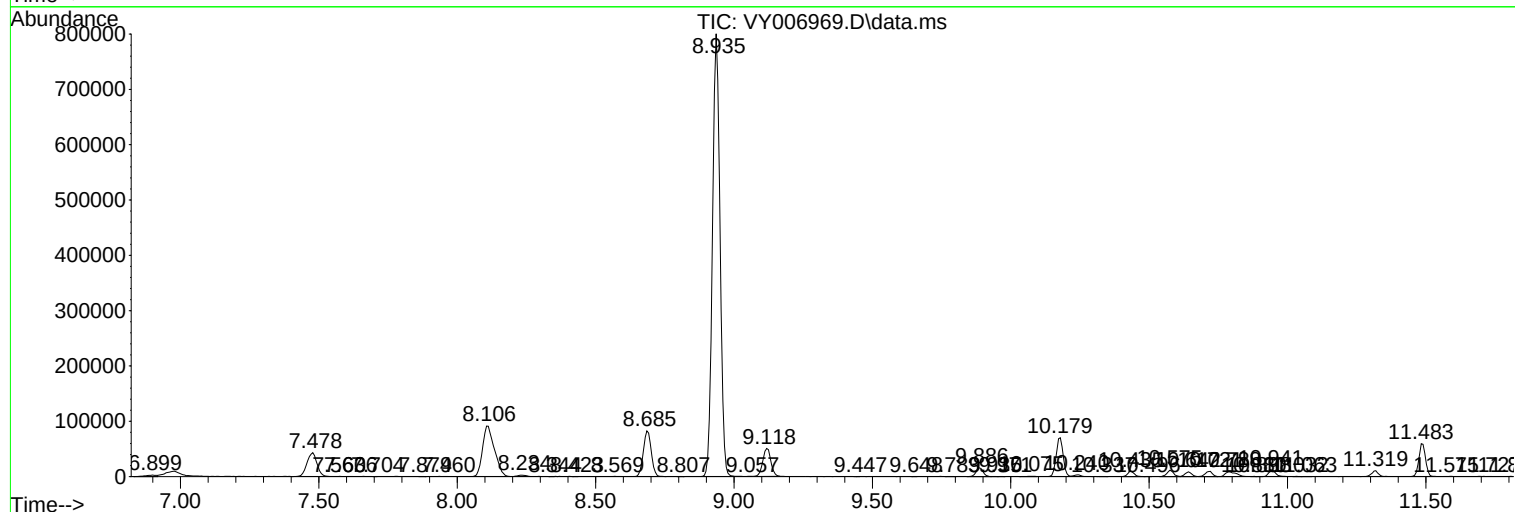
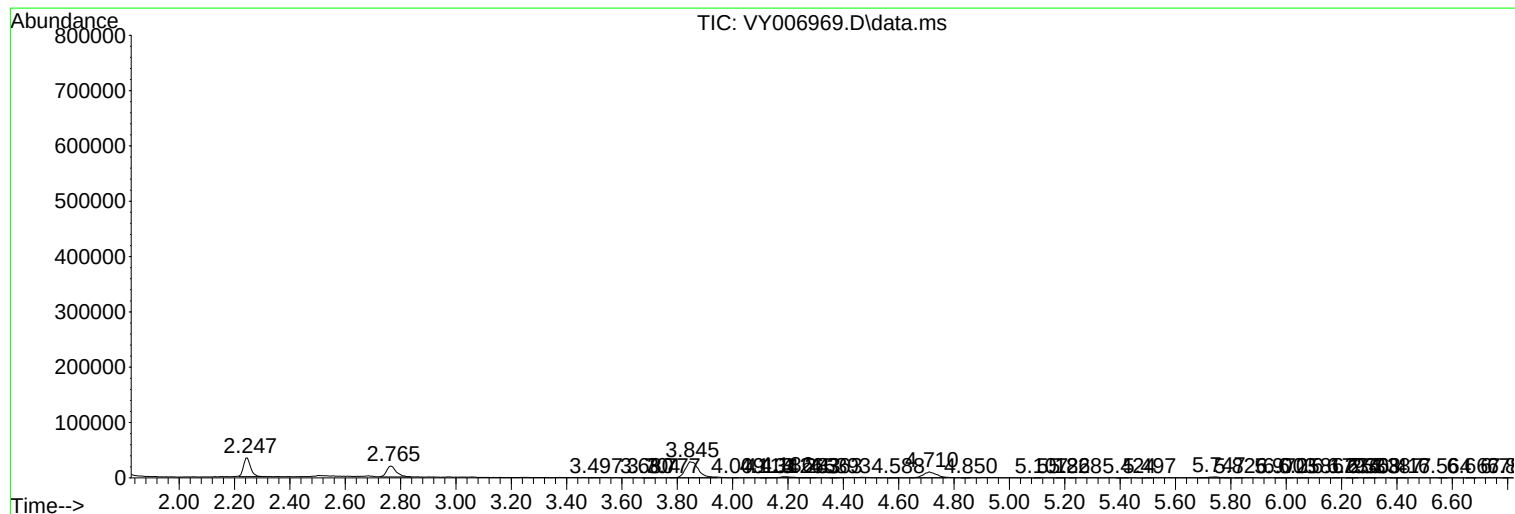
Sum of corrected areas: 3042525

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MSVOA_Y
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EX8C9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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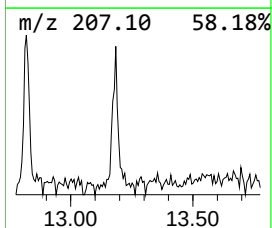
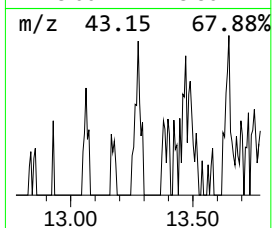
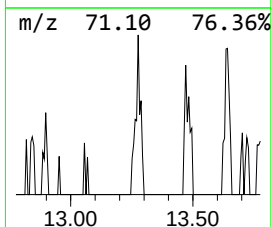
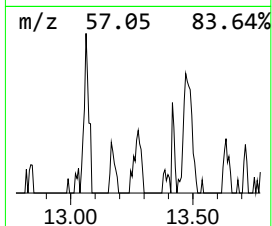
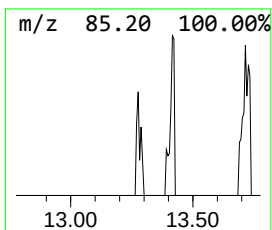
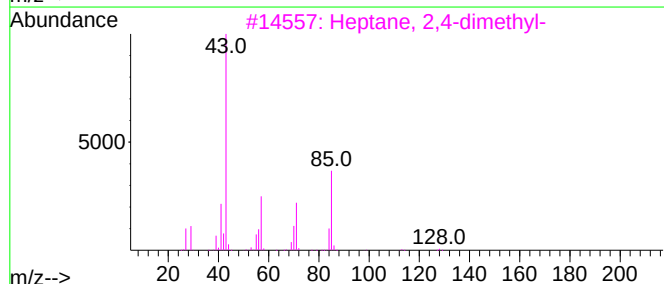
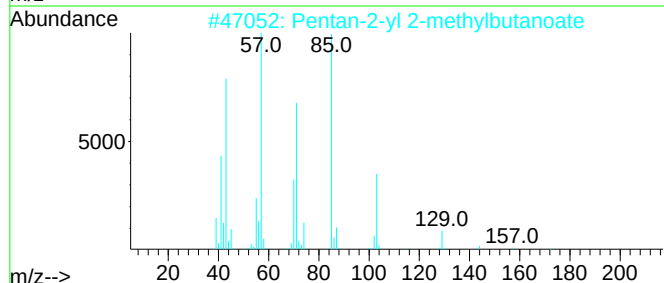
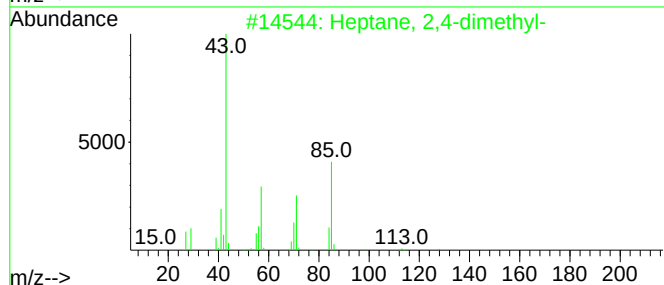
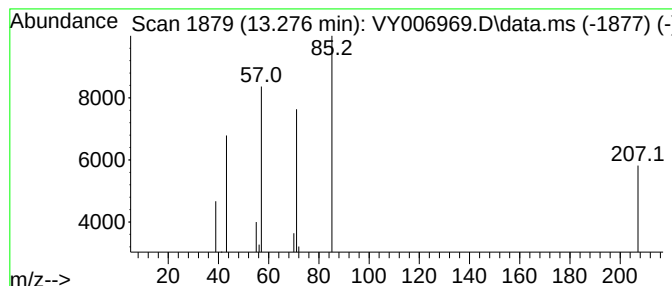
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLEM120321SMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.276	1.38 ug/L	1955	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
2			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	45
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	45
4			Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	42
5			Sulfurous acid, isohexyl 2-penty...	236	C11H24O3S	1000309-15-5	42



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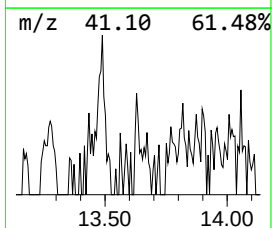
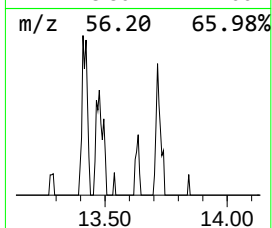
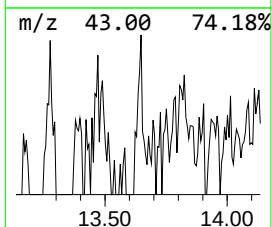
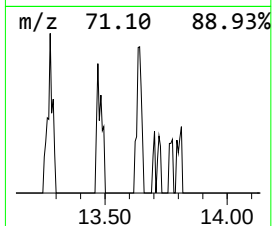
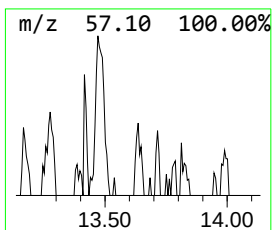
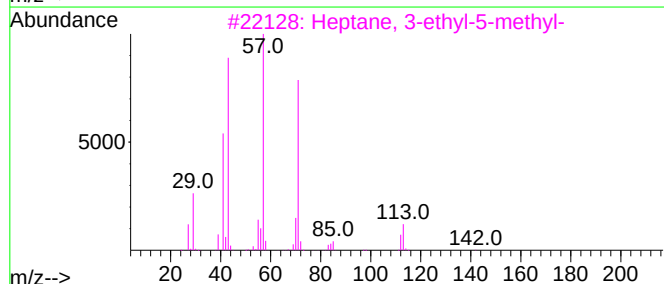
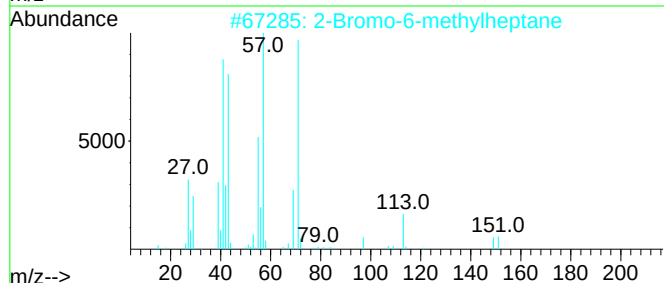
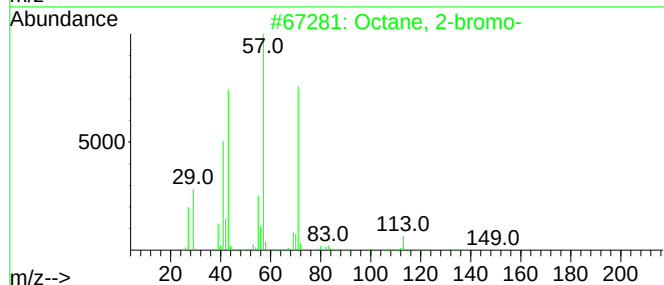
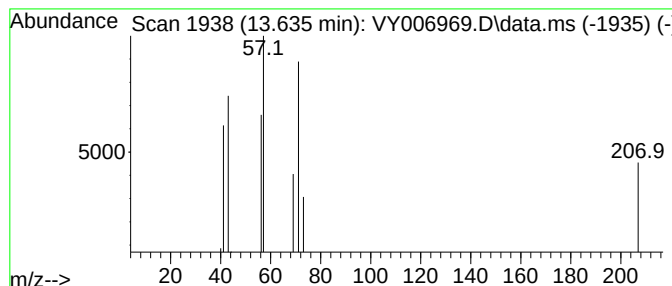
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TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown-01 Concentration Rank 9

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13.636	1.43 ug/L	2022	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-			192	C8H17Br	000557-35-7	9
2	2-Bromo-6-methylheptane			192	C8H17Br	004730-24-9	9
3	Heptane, 3-ethyl-5-methyl-			142	C10H22	052896-90-9	9
4	Butane, 2,2-dimethyl-			86	C6H14	000075-83-2	9
5	Azetidine			57	C3H7N	000503-29-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	13.276	1.4	ug/L	1955	3	13.422	35412	25.0
unknown-01	13.636	1.4	ug/L	2022	3	13.422	35412	25.0