

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
 Data File : VU055824.D
 Acq On : 20 Oct 2023 11:34
 Operator : MD/SY
 Sample : 04947-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E45J2

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_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.490	56	62	67	rBV4	8607	10238	0.01%	0.003%
2	1.602	88	97	116	rBV2	967428	1186130	0.74%	0.405%
3	1.892	179	187	205	rVB	187028	275619	0.17%	0.094%
4	1.975	206	213	223	rVB	43100	64167	0.04%	0.022%
5	2.194	273	281	288	rBV3	15713	22339	0.01%	0.008%
6	2.560	382	395	414	rBV2	427816	721802	0.45%	0.246%
7	2.711	438	442	450	rVB6	1250	1202	0.00%	0.000%
8	2.773	457	461	463	rBV4	823	705	0.00%	0.000%
9	2.956	511	518	520	rBV3	704	543	0.00%	0.000%
10	2.965	520	521	528	rVB3	384	240	0.00%	0.000%
11	3.039	532	544	550	rBV6	6484	13065	0.01%	0.004%
12	3.129	564	572	579	rBV5	2770	4197	0.00%	0.001%
13	3.226	599	602	606	rVB2	629	400	0.00%	0.000%
14	3.345	625	639	664	rVV	316647	635655	0.40%	0.217%
15	3.547	699	702	705	rBV2	524	301	0.00%	0.000%
16	3.583	710	713	716	rBV5	759	524	0.00%	0.000%
17	3.650	731	734	738	rBV2	366	235	0.00%	0.000%
18	3.689	738	746	756	rVV5	1904	3441	0.00%	0.001%
19	3.744	760	763	768	rVB	421	338	0.00%	0.000%
20	3.769	768	771	775	rVB2	465	350	0.00%	0.000%
21	3.814	780	785	788	rBV2	513	511	0.00%	0.000%
22	3.978	833	836	837	rBV3	800	453	0.00%	0.000%
23	4.168	891	895	898	rBV2	397	398	0.00%	0.000%
24	4.393	963	965	969	rVB	646	388	0.00%	0.000%
25	4.416	969	972	975	rBV2	309	267	0.00%	0.000%
26	4.432	975	977	981	rBV4	618	457	0.00%	0.000%
27	4.525	993	1006	1019	rVB5	5562	11586	0.01%	0.004%
28	4.657	1023	1047	1076	rBV	20262880	45670091	28.44%	15.592%
29	5.055	1158	1171	1198	rVB2	382504	838896	0.52%	0.286%
30	5.322	1250	1254	1261	rVB5	1431	1601	0.00%	0.001%
31	5.467	1294	1299	1306	rVB6	1241	1552	0.00%	0.001%
32	5.515	1309	1314	1315	rBV2	520	344	0.00%	0.000%
33	5.547	1321	1324	1328	rBV4	576	522	0.00%	0.000%
34	5.589	1334	1337	1339	rVB3	613	345	0.00%	0.000%
35	5.608	1339	1343	1346	rBV4	629	554	0.00%	0.000%
36	5.718	1356	1377	1404	rBV2	762619	2110847	1.31%	0.721%

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 Title : VOC Analysis

37	5.972	1451	1456	1460	rBV5	1389	1480	0.00%	0.001%
38	6.030	1470	1474	1478	rVB3	924	710	0.00%	0.000%
39	6.107	1493	1498	1501	rBV4	452	422	0.00%	0.000%
40	6.245	1525	1541	1561	rBV	604362	1174714	0.73%	0.401%
41	6.538	1614	1632	1668	rBV	36618399	69918836	43.53%	23.871%
42	6.686	1670	1678	1709	rVB	503502	1019777	0.63%	0.348%
43	7.030	1783	1785	1790	rVB4	1185	652	0.00%	0.000%
44	7.104	1805	1808	1810	rBV2	861	521	0.00%	0.000%
45	7.152	1816	1823	1826	rBV4	1014	1265	0.00%	0.000%
46	7.190	1826	1835	1842	rBV4	7228	12921	0.01%	0.004%
47	7.332	1876	1879	1882	rVB5	532	357	0.00%	0.000%
48	7.499	1929	1931	1933	rBV3	617	276	0.00%	0.000%
49	7.560	1938	1950	1979	rVV	263191	474221	0.30%	0.162%
50	7.692	1985	1991	1993	rBV6	3713	3609	0.00%	0.001%
51	7.798	2019	2024	2028	rBV4	800	880	0.00%	0.000%
52	7.817	2028	2030	2033	rVB3	579	309	0.00%	0.000%
53	7.840	2033	2037	2040	rBV4	751	532	0.00%	0.000%
54	7.895	2040	2054	2071	rBV	966539	1666105	1.04%	0.569%
55	8.091	2113	2115	2121	rVB4	722	521	0.00%	0.000%
56	8.177	2130	2142	2163	rBV	179873	315135	0.20%	0.108%
57	8.306	2180	2182	2185	rVB3	478	223	0.00%	0.000%
58	8.377	2201	2204	2207	rBV2	480	312	0.00%	0.000%
59	8.399	2207	2211	2218	rVB7	1315	1683	0.00%	0.001%
60	8.435	2218	2222	2224	rBV3	647	382	0.00%	0.000%
61	8.470	2231	2233	2236	rVB4	577	270	0.00%	0.000%
62	8.560	2241	2261	2277	rBV4	83394311	160604598	100.00%	54.831%
63	9.280	2475	2485	2506	rVB2	72302	125719	0.08%	0.043%
64	9.412	2514	2526	2555	rBV	921566	1573831	0.98%	0.537%
65	10.087	2733	2736	2737	rBV3	1212	685	0.00%	0.000%
66	10.287	2795	2798	2801	rBV2	794	522	0.00%	0.000%
67	10.354	2815	2819	2822	rBV4	1116	1284	0.00%	0.000%
68	10.386	2828	2829	2832	rVB3	573	238	0.00%	0.000%
69	10.444	2843	2847	2850	rBV3	667	593	0.00%	0.000%
70	10.547	2877	2879	2883	rBV3	456	328	0.00%	0.000%
71	10.753	2929	2943	2964	rBV	728102	1211632	0.75%	0.414%
72	11.020	3024	3026	3029	rBV	586	353	0.00%	0.000%
73	11.062	3035	3039	3043	rBV3	754	716	0.00%	0.000%
74	11.158	3066	3069	3071	rBV	460	310	0.00%	0.000%
75	11.232	3089	3092	3094	rBV	389	273	0.00%	0.000%
76	11.245	3094	3096	3099	rVV2	403	257	0.00%	0.000%

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77	11.290	3108	3110	3116	rVB4	547	488	0.00%	0.000%
78	11.386	3134	3140	3144	rBV5	1881	2157	0.00%	0.001%
79	11.438	3152	3156	3161	rVB5	638	534	0.00%	0.000%
80	11.470	3161	3166	3168	rBV2	1531	1388	0.00%	0.000%
81	11.509	3175	3178	3182	rBV3	572	430	0.00%	0.000%
82	11.544	3186	3189	3190	rBV2	637	330	0.00%	0.000%
83	11.701	3229	3238	3240	rBV8	3565	4750	0.00%	0.002%
84	11.808	3259	3271	3294	rBV	958929	1558890	0.97%	0.532%
85	12.094	3353	3360	3361	rBV4	2416	2218	0.00%	0.001%
86	12.190	3376	3390	3413	rBV	965386	1625632	1.01%	0.555%
87	12.322	3429	3431	3441	rVB5	1255	1389	0.00%	0.000%
88	12.412	3457	3459	3463	rBV2	508	396	0.00%	0.000%
89	12.515	3490	3491	3495	rBV3	520	315	0.00%	0.000%
90	12.627	3523	3526	3531	rBV4	577	558	0.00%	0.000%
91	12.714	3551	3553	3558	rVB3	599	396	0.00%	0.000%
92	12.737	3558	3560	3562	rBV2	738	409	0.00%	0.000%
93	12.756	3562	3566	3568	rBV3	641	548	0.00%	0.000%
94	12.891	3606	3608	3610	rBV3	685	413	0.00%	0.000%
95	12.910	3611	3614	3620	rVV5	1770	2031	0.00%	0.001%
96	13.377	3757	3759	3763	rBV3	643	543	0.00%	0.000%
97	13.570	3815	3819	3821	rBV3	680	601	0.00%	0.000%
98	13.598	3826	3828	3831	rBV2	672	385	0.00%	0.000%
99	13.856	3904	3908	3918	rVB6	2342	3449	0.00%	0.001%
100	14.280	4038	4040	4044	rVB3	660	329	0.00%	0.000%

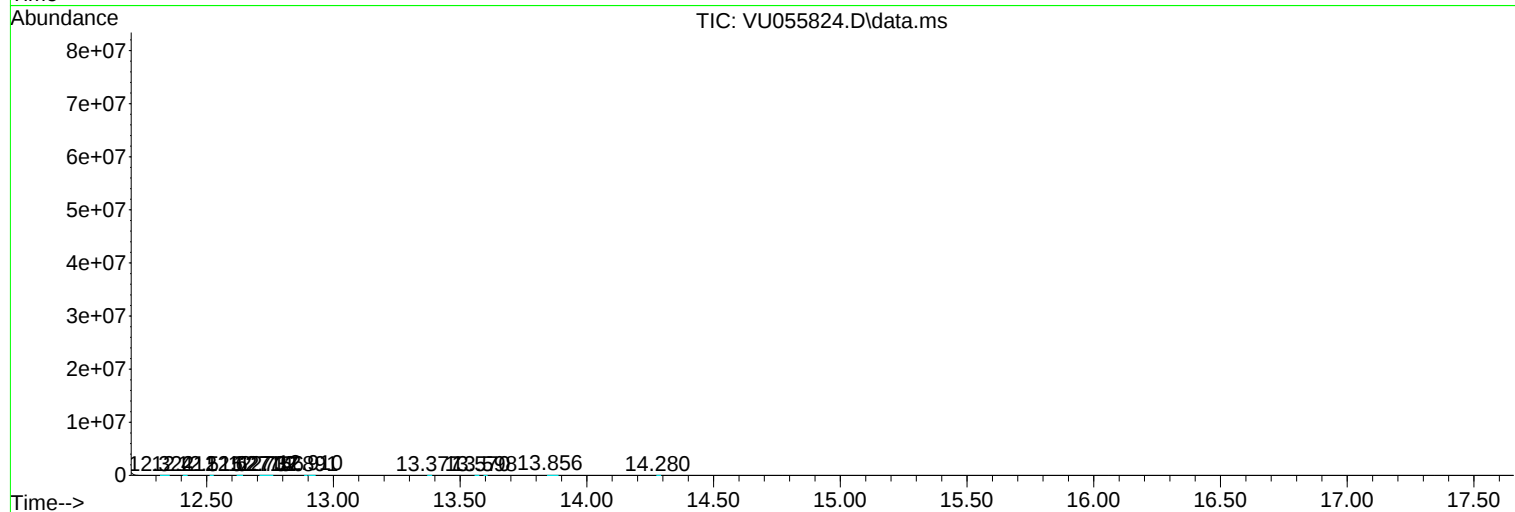
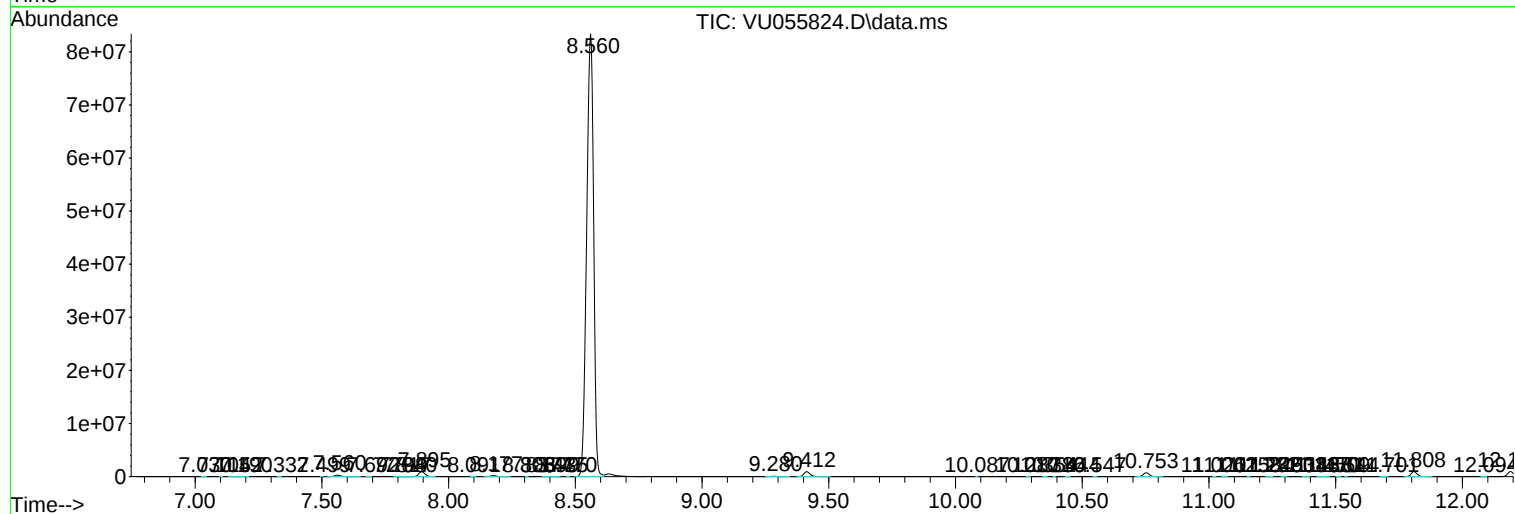
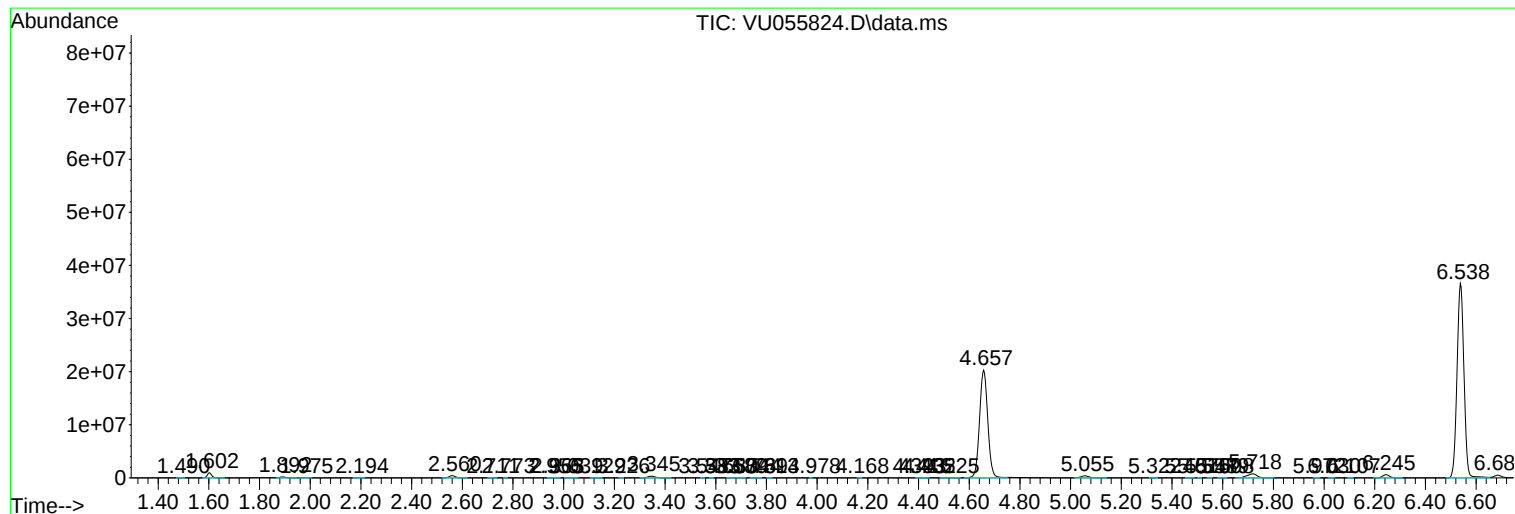
Sum of corrected areas: 292906334

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Quant Title : VOC Analysis

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



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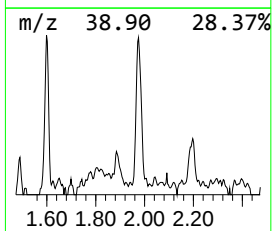
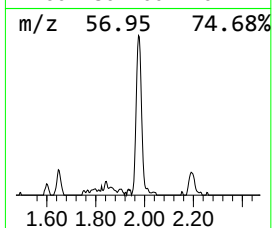
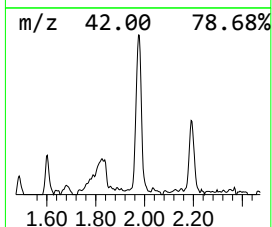
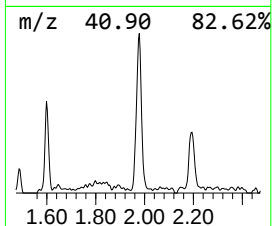
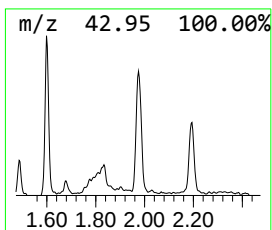
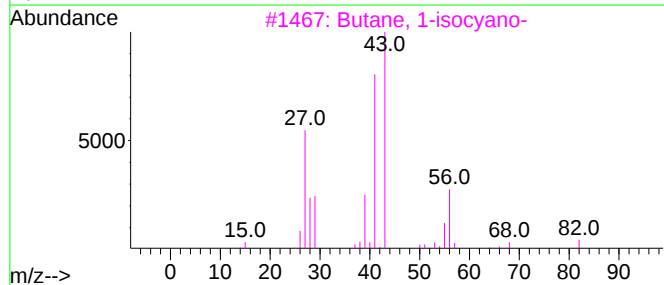
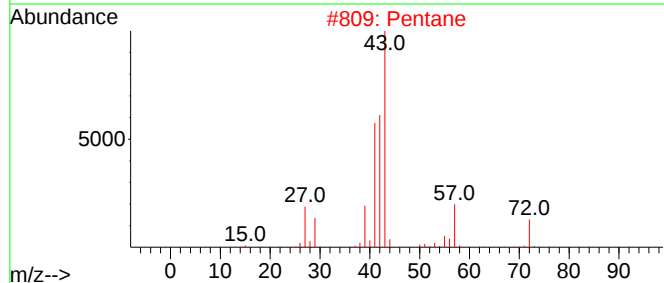
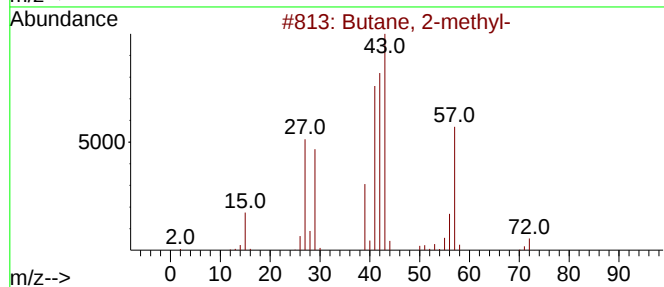
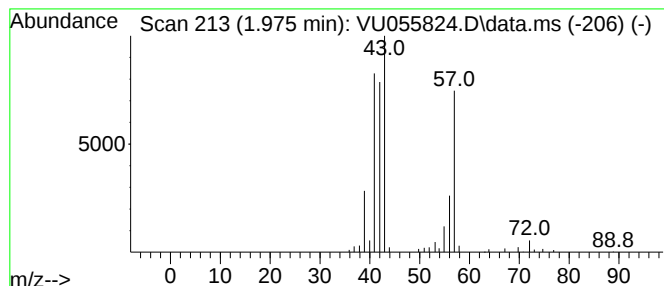
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.975	2.73 ug/L	64167	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	80
2		Pentane	72	C5H12	000109-66-0	33
3		Butane, 1-isocyano-	83	C5H9N	002769-64-4	27
4		1-Pentene	70	C5H10	000109-67-1	23
5		1-Butene	56	C4H8	000106-98-9	18



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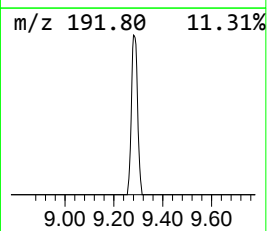
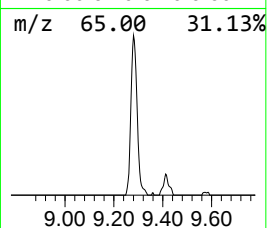
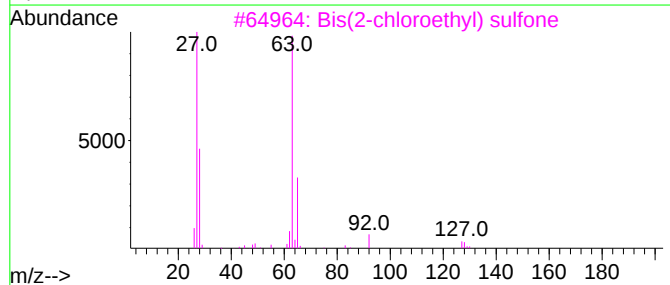
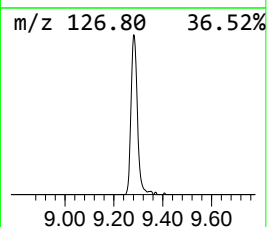
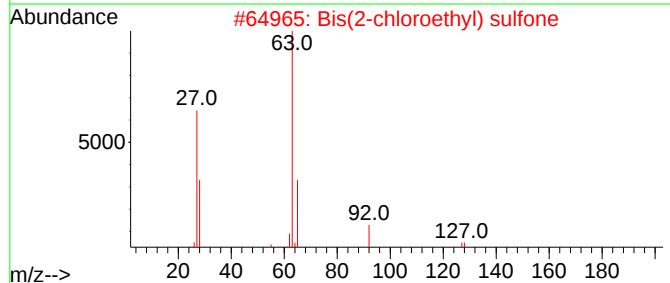
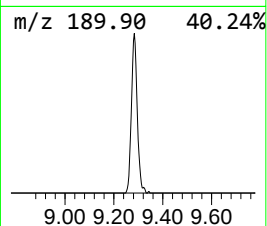
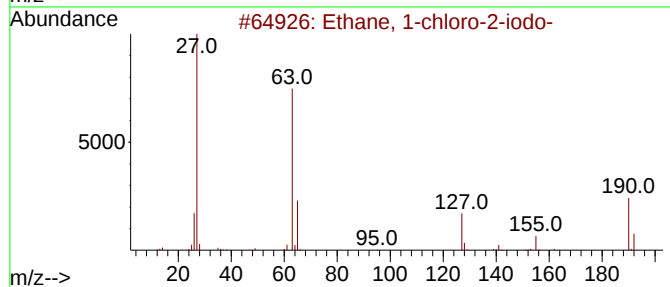
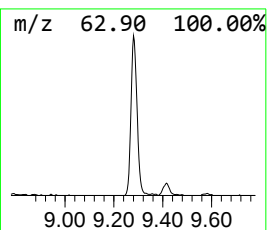
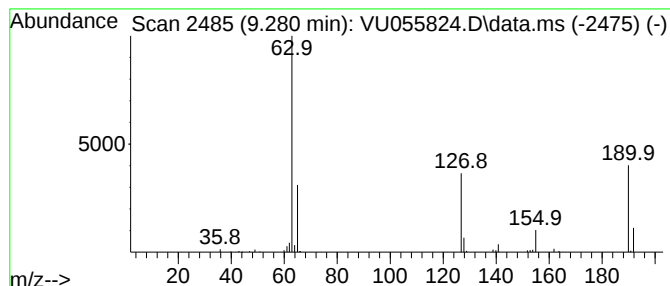
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethane, 1-chloro-2-iodo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.280	3.99 ug/L	125719	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-2-iodo-	190	C2H4ClI	000624-70-4	91
2			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	39
3			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	38
4			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	38
5			Ethane, 1-bromo-2-chloro-	142	C2H4BrCl	000107-04-0	38



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.975	2.7	ug/L	64167	1	6.245	1174710	50.0
Ethane, 1-chlor...	9.280	4.0	ug/L	125719	2	9.412	1573830	50.0