

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037488.D
 Acq On : 23 Sep 2024 17:21
 Operator : SY/MD
 Sample : P4106-01
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0SX5

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_V\Method\SFAMVLM082624WMA.M

Title : VOC Analysis

Signal : TIC: VV037488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	34	41	53	rBV	76594	117596	1.45%	0.350%
2	1.278	67	74	91	rVB	421913	451436	5.56%	1.345%
3	1.384	104	107	112	rBV	8486	6734	0.08%	0.020%
4	1.532	145	153	168	rVB	360986	419634	5.17%	1.250%
5	2.060	307	317	328	rBV	729304	1052873	12.97%	3.137%
6	2.558	465	472	490	rVB	35759	72099	0.89%	0.215%
7	3.333	711	713	717	rVB4	1171	630	0.01%	0.002%
8	3.507	764	767	769	rBV3	820	559	0.01%	0.002%
9	3.561	780	784	787	rBV4	947	914	0.01%	0.003%
10	3.587	789	792	796	rBV3	1301	815	0.01%	0.002%
11	3.626	796	804	818	rBV4	10622	26449	0.33%	0.079%
12	3.754	842	844	847	rVV3	1204	888	0.01%	0.003%
13	3.793	847	856	905	rVV2	158255	525648	6.48%	1.566%
14	4.243	977	996	1025	rBV	496160	1263863	15.57%	3.766%
15	4.471	1064	1067	1069	rBV4	944	487	0.01%	0.001%
16	4.494	1069	1074	1076	rBV5	788	692	0.01%	0.002%
17	4.542	1084	1089	1091	rBV4	1656	1270	0.02%	0.004%
18	4.587	1097	1103	1107	rBV7	807	977	0.01%	0.003%
19	4.629	1113	1116	1119	rBV4	809	546	0.01%	0.002%
20	4.677	1127	1131	1135	rVB5	849	753	0.01%	0.002%
21	4.712	1138	1142	1145	rBV5	988	634	0.01%	0.002%
22	4.751	1152	1154	1158	rBV5	1129	718	0.01%	0.002%
23	4.847	1180	1184	1188	rVB5	826	851	0.01%	0.003%
24	4.950	1198	1216	1253	rBV2	1240573	3181928	39.20%	9.481%
25	5.220	1296	1300	1302	rBV5	845	554	0.01%	0.002%
26	5.307	1324	1327	1329	rBV3	824	513	0.01%	0.002%
27	5.362	1341	1344	1352	rVB8	910	999	0.01%	0.003%
28	5.397	1352	1355	1359	rBV6	1475	1218	0.02%	0.004%
29	5.436	1363	1367	1370	rBV5	1297	1008	0.01%	0.003%
30	5.465	1374	1376	1380	rVB4	1325	774	0.01%	0.002%
31	5.529	1383	1396	1432	rBV	954815	1954211	24.07%	5.823%
32	5.751	1463	1465	1472	rVB7	1212	1056	0.01%	0.003%
33	5.834	1476	1491	1493	rBV7	6549	11465	0.14%	0.034%
34	5.896	1508	1510	1513	rBV3	715	563	0.01%	0.002%
35	5.982	1524	1537	1572	rBV	683833	1423593	17.54%	4.242%
36	6.359	1651	1654	1657	rBV4	929	570	0.01%	0.002%

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 Title : VOC Analysis

37	6.388	1661	1663	1665	rBV3	1198	749	0.01%	0.002%
38	6.400	1665	1667	1673	rVB5	1388	1206	0.01%	0.004%
39	6.484	1691	1693	1697	rBV4	1055	883	0.01%	0.003%
40	6.551	1710	1714	1717	rVB4	753	623	0.01%	0.002%
41	6.571	1717	1720	1722	rBV4	1032	612	0.01%	0.002%
42	6.661	1743	1748	1750	rBV5	841	858	0.01%	0.003%
43	6.699	1757	1760	1763	rVB4	836	554	0.01%	0.002%
44	6.773	1778	1783	1785	rVB5	862	645	0.01%	0.002%
45	6.908	1814	1825	1853	rBV	378684	721080	8.88%	2.149%
46	7.236	1915	1927	1968	rBV	1450309	2563668	31.58%	7.639%
47	7.500	2006	2009	2011	rBV4	925	605	0.01%	0.002%
48	7.548	2015	2024	2057	rVV	246600	460336	5.67%	1.372%
49	7.815	2101	2107	2110	rVB6	1321	1061	0.01%	0.003%
50	7.844	2114	2116	2117	rBV	1246	575	0.01%	0.002%
51	7.879	2124	2127	2130	rVB5	1733	1080	0.01%	0.003%
52	7.966	2148	2154	2156	rBV4	764	679	0.01%	0.002%
53	7.986	2156	2160	2162	rBV5	1246	1004	0.01%	0.003%
54	8.024	2162	2172	2208	rBV	501811	987995	12.17%	2.944%
55	8.719	2382	2388	2395	rBV7	1756	2333	0.03%	0.007%
56	8.780	2395	2407	2440	rBV2	1474941	3144459	38.74%	9.369%
57	9.143	2510	2520	2536	rVB2	5613	12723	0.16%	0.038%
58	9.249	2548	2553	2554	rBV5	660	524	0.01%	0.002%
59	9.297	2564	2568	2570	rBV3	1127	871	0.01%	0.003%
60	9.375	2589	2592	2595	rVB4	1302	715	0.01%	0.002%
61	9.403	2597	2601	2602	rBV4	1550	767	0.01%	0.002%
62	9.484	2621	2626	2628	rBV6	1148	1002	0.01%	0.003%
63	9.638	2667	2674	2675	rBV4	2831	3004	0.04%	0.009%
64	9.712	2694	2697	2700	rBV4	891	914	0.01%	0.003%
65	9.731	2700	2703	2709	rVV6	1279	1467	0.02%	0.004%
66	9.783	2715	2719	2725	rVB7	2087	1649	0.02%	0.005%
67	9.838	2732	2736	2739	rBV5	903	686	0.01%	0.002%
68	9.854	2739	2741	2744	rVV5	1335	943	0.01%	0.003%
69	9.905	2754	2757	2760	rBV5	785	723	0.01%	0.002%
70	9.953	2770	2772	2777	rVB5	2370	1589	0.02%	0.005%
71	10.002	2783	2787	2788	rBV4	1955	1294	0.02%	0.004%
72	10.146	2820	2832	2850	rBV	803466	1272211	15.67%	3.791%
73	10.291	2872	2877	2878	rBV4	1768	1428	0.02%	0.004%
74	10.381	2900	2905	2906	rBV4	3815	3222	0.04%	0.010%
75	10.513	2940	2946	2957	rVB3	26803	38712	0.48%	0.115%
76	10.635	2981	2984	2986	rBV4	1192	779	0.01%	0.002%

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 Title : VOC Analysis

77	10.680	2995	2998	3000	rBV3	1842	1238	0.02%	0.004%
78	10.764	3021	3024	3025	rBV3	1747	1018	0.01%	0.003%
79	10.812	3032	3039	3046	rBV6	7883	10692	0.13%	0.032%
80	10.973	3084	3089	3094	rBV9	3897	4513	0.06%	0.013%
81	11.114	3124	3133	3143	rBV	122105	201807	2.49%	0.601%
82	11.178	3143	3153	3177	rVV2	1589565	2772524	34.16%	8.261%
83	11.397	3217	3221	3230	rVB6	11379	15459	0.19%	0.046%
84	11.432	3230	3232	3239	rVB8	2554	1968	0.02%	0.006%
85	11.487	3240	3249	3256	rBV4	19112	39844	0.49%	0.119%
86	11.571	3259	3275	3300	rVV2	4059552	8117353	100.00%	24.186%
87	11.725	3316	3323	3330	rBV2	51313	66548	0.82%	0.198%
88	11.844	3357	3360	3362	rBV4	5215	3957	0.05%	0.012%
89	12.400	3527	3533	3539	rBV8	8979	12024	0.15%	0.036%
90	12.439	3541	3545	3553	rVB7	8830	11682	0.14%	0.035%
91	12.577	3581	3588	3603	rVB	37639	65556	0.81%	0.195%
92	12.825	3657	3665	3679	rVB	36678	56029	0.69%	0.167%
93	13.191	3768	3779	3809	rBV	700484	1128028	13.90%	3.361%
94	13.323	3814	3820	3826	rBV4	17362	23749	0.29%	0.071%
95	13.673	3919	3929	3947	rVB	354244	560038	6.90%	1.669%
96	13.837	3974	3980	3987	rVB2	31152	37535	0.46%	0.112%
97	14.844	4288	4293	4312	rVB3	43181	76981	0.95%	0.229%
98	15.329	4437	4444	4458	rVB2	70601	128221	1.58%	0.382%
99	15.779	4577	4584	4598	rVB	253888	372298	4.59%	1.109%
100	16.213	4714	4719	4733	rVB3	61513	90813	1.12%	0.271%

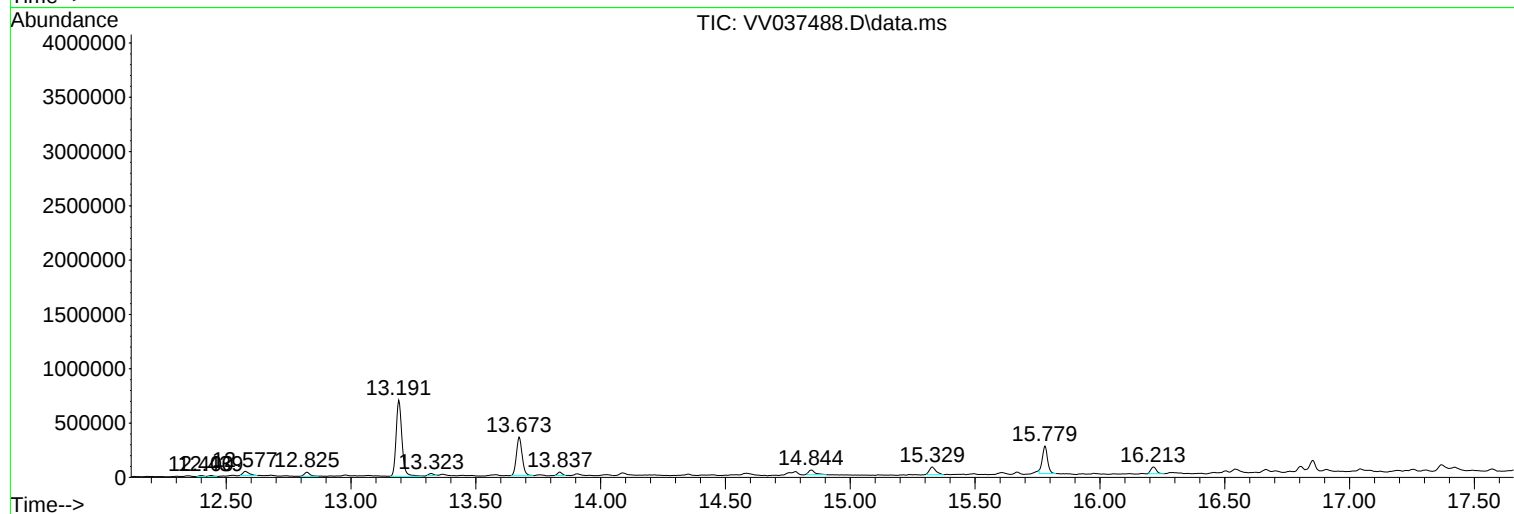
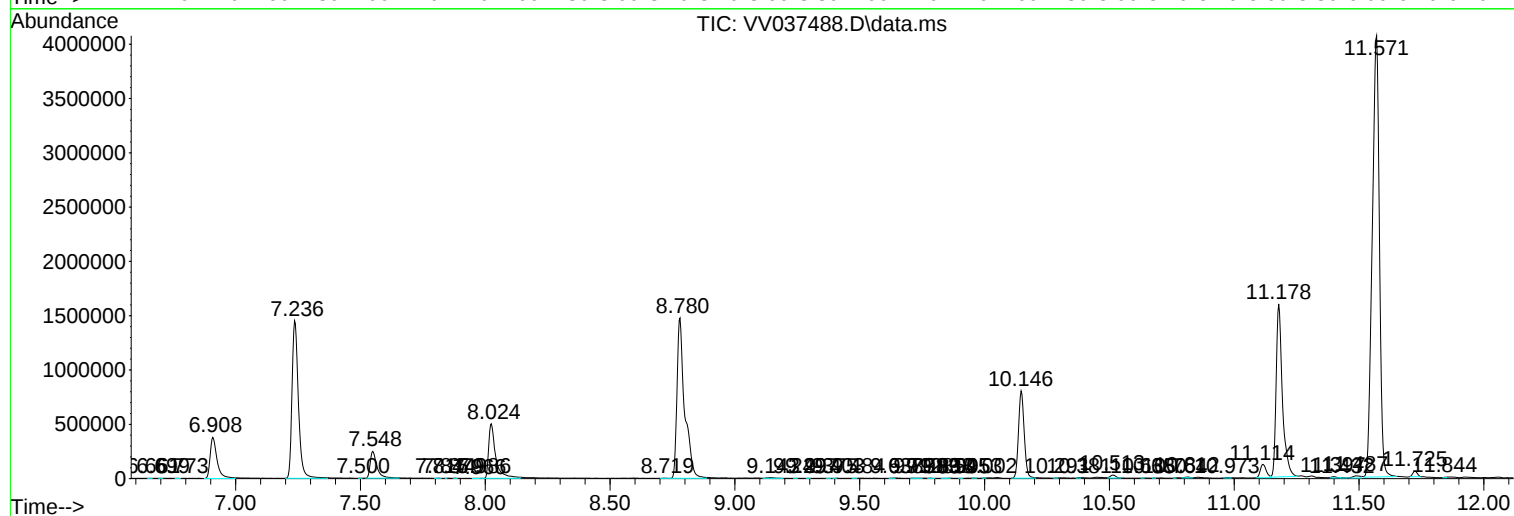
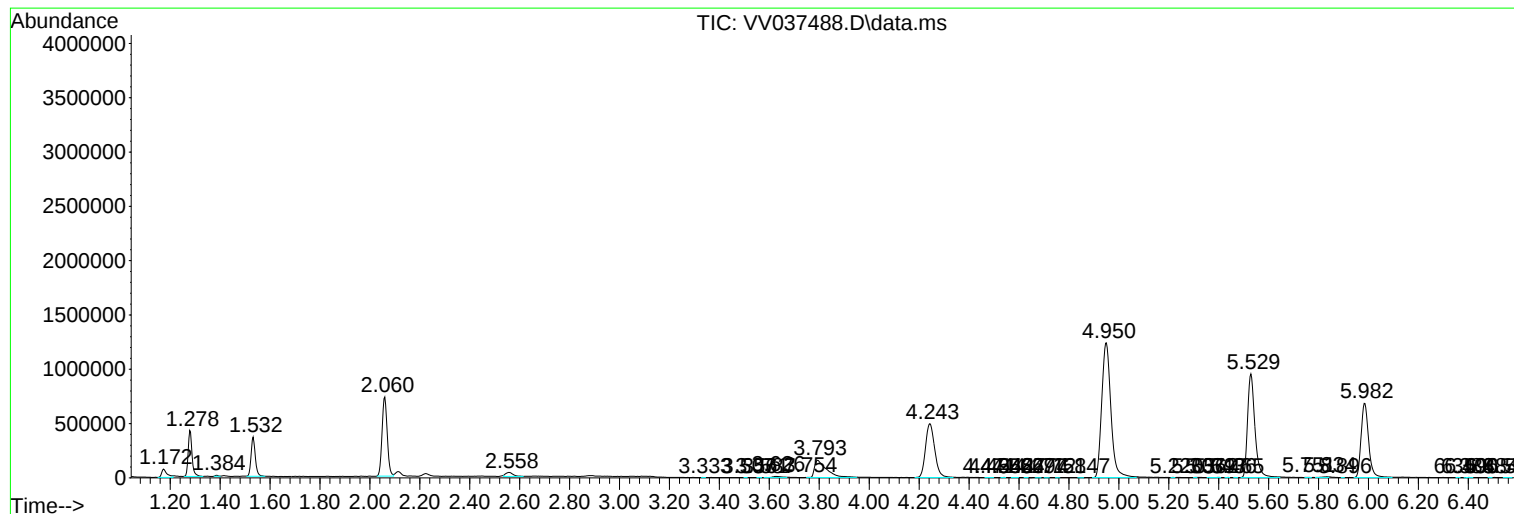
Sum of corrected areas: 33561621

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MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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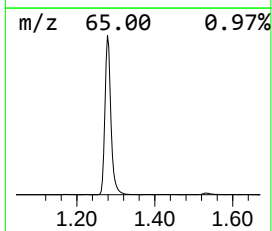
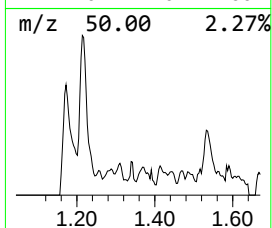
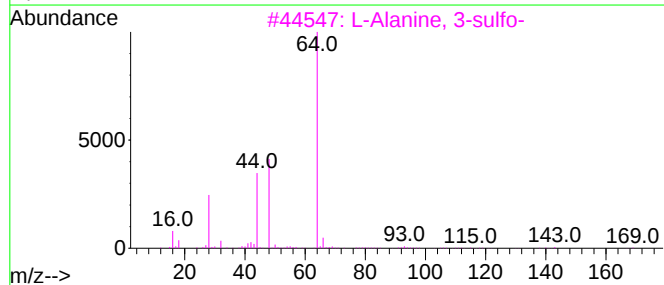
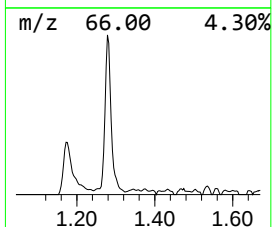
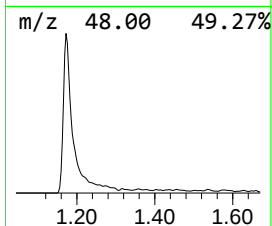
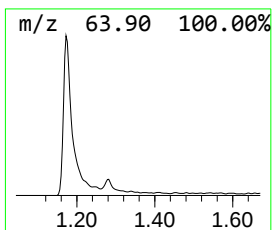
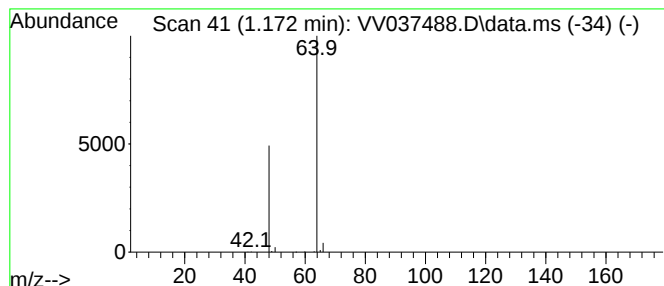
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.172	3.01 ug/L	117596	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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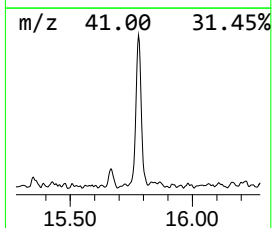
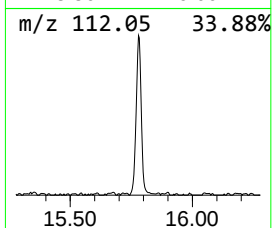
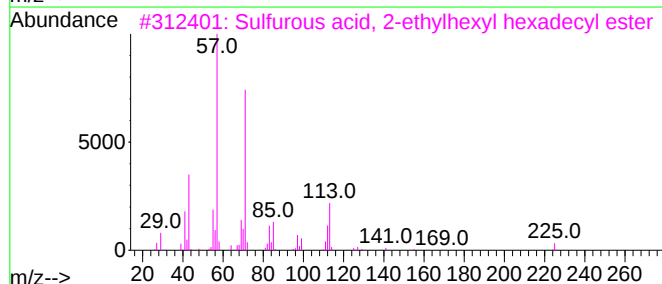
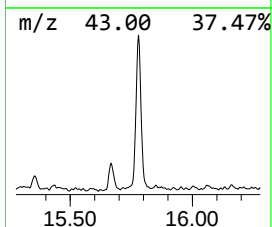
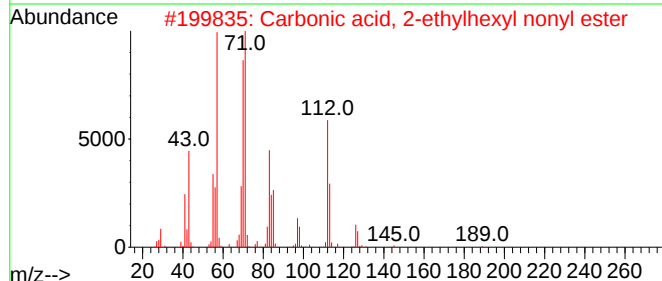
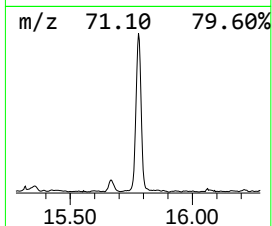
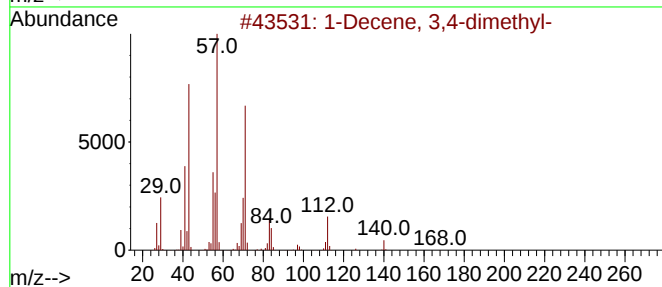
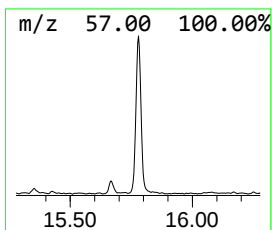
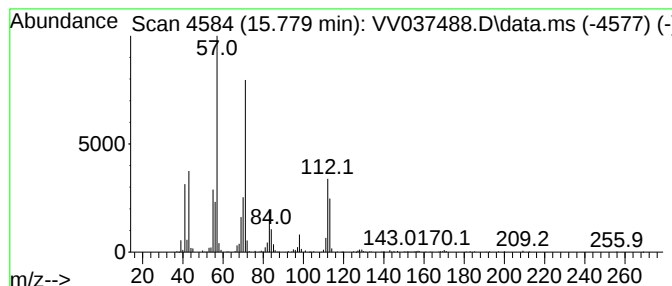
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.779	6.71 ug/L	372298	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 3,4-dimethyl-			168	C12H24	050871-03-9	72
2	Carbonic acid, 2-ethylhexyl nony...			300	C18H36O3	1000383-13-6	64
3	Sulfurous acid, 2-ethylhexyl hex...			418	C24H50O3S	1000309-19-9	64
4	Octane, 1,1'-oxybis-			242	C16H34O	000629-82-3	64
5	Dodecane, 2,6,11-trimethyl-			212	C15H32	031295-56-4	62



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.172	3.0	ug/L	117596	1	5.529	1954210	50.0
(DEL) Alkane: S...	15.779	6.7	ug/L	372298	3	11.178	2772520	50.0