

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
 Data File : VV037662.D
 Acq On : 30 Sep 2024 17:46
 Operator : SY/MD
 Sample : P4162-21ME
 Misc : 4.91g/5mL/100ul/5mL/MSVOA_V/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A4EJ6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M

Title : VOC Analysis

Signal : TIC: VV037662.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.188	37	46	49	rBV3	8209	10675	0.39%	0.050%
2	1.211	49	53	60	rVV2	6766	9082	0.33%	0.043%
3	1.278	66	74	93	rBV	253676	316264	11.56%	1.492%
4	1.468	110	133	135	rBV7	40346	109601	4.01%	0.517%
5	1.507	140	145	156	rVB	146262	194050	7.09%	0.915%
6	1.767	224	226	228	rBV3	1957	1150	0.04%	0.005%
7	1.976	287	291	293	rBV5	1468	1333	0.05%	0.006%
8	2.044	301	312	331	rBV	553811	814245	29.76%	3.841%
9	2.378	408	416	426	rVB	8152	14069	0.51%	0.066%
10	2.552	458	470	484	rBV	12133	26673	0.98%	0.126%
11	2.748	528	531	535	rVB6	1971	1134	0.04%	0.005%
12	2.812	549	551	555	rVV5	1299	960	0.04%	0.005%
13	2.860	563	566	569	rBV5	1553	1287	0.05%	0.006%
14	2.982	602	604	610	rVB6	1947	1504	0.05%	0.007%
15	3.198	668	671	675	rVB5	961	714	0.03%	0.003%
16	3.638	801	808	811	rBV4	881	1328	0.05%	0.006%
17	3.709	827	830	834	rVB3	897	729	0.03%	0.003%
18	3.802	850	859	900	rBV2	89096	371941	13.60%	1.755%
19	4.240	977	995	1035	rBV2	421534	1140944	41.71%	5.382%
20	4.625	1112	1115	1121	rVB5	835	757	0.03%	0.004%
21	4.809	1168	1172	1177	rBV4	965	904	0.03%	0.004%
22	4.944	1199	1214	1256	rBV2	1051577	2735611	100.00%	12.905%
23	5.088	1256	1259	1264	rVB6	1821	1700	0.06%	0.008%
24	5.137	1271	1274	1276	rBV3	1475	748	0.03%	0.004%
25	5.269	1313	1315	1319	rBV3	953	807	0.03%	0.004%
26	5.326	1330	1333	1337	rVB5	895	736	0.03%	0.003%
27	5.410	1356	1359	1362	rBV4	1405	903	0.03%	0.004%
28	5.526	1384	1395	1433	rBV	719636	1570285	57.40%	7.408%
29	5.831	1477	1490	1506	rBV8	9815	23662	0.86%	0.112%
30	5.982	1523	1537	1573	rVV	589521	1276045	46.65%	6.020%
31	6.140	1584	1586	1595	rVB9	2097	1863	0.07%	0.009%
32	6.378	1656	1660	1664	rBV5	973	896	0.03%	0.004%
33	6.452	1677	1683	1685	rBV5	720	759	0.03%	0.004%
34	6.603	1726	1730	1732	rVB4	1145	763	0.03%	0.004%
35	6.715	1759	1765	1767	rBV4	840	681	0.02%	0.003%
36	6.908	1814	1825	1850	rBV2	317965	633669	23.16%	2.989%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SFAMVLM092624WMA.M
 Title : VOC Analysis

37	7.236	1915	1927	1947	rBV	1186927	2158437	78.90%	10.182%
38	7.445	1989	1992	1996	rVB6	1755	1168	0.04%	0.006%
39	7.503	2008	2010	2014	rVB5	1890	1276	0.05%	0.006%
40	7.551	2014	2025	2054	rBV	212413	426912	15.61%	2.014%
41	7.767	2089	2092	2096	rBV6	754	713	0.03%	0.003%
42	7.870	2118	2124	2127	rVV6	1029	1055	0.04%	0.005%
43	7.973	2154	2156	2162	rVB4	1703	1178	0.04%	0.006%
44	8.034	2165	2175	2204	rBV3	331585	869139	31.77%	4.100%
45	8.368	2275	2279	2291	rVB7	2663	3900	0.14%	0.018%
46	8.452	2301	2305	2310	rVB8	1055	875	0.03%	0.004%
47	8.551	2330	2336	2339	rBV7	1372	1385	0.05%	0.007%
48	8.667	2368	2372	2374	rBV2	867	715	0.03%	0.003%
49	8.780	2395	2407	2444	rBV	1148189	1959911	71.64%	9.246%
50	9.040	2481	2488	2489	rBV6	1026	1112	0.04%	0.005%
51	9.050	2489	2491	2495	rVV4	1023	726	0.03%	0.003%
52	9.301	2565	2569	2575	rVB7	1080	1082	0.04%	0.005%
53	9.339	2575	2581	2584	rBV7	783	788	0.03%	0.004%
54	9.365	2584	2589	2591	rBV4	842	817	0.03%	0.004%
55	9.381	2591	2594	2597	rVV4	1722	1289	0.05%	0.006%
56	9.458	2614	2618	2621	rVB3	1107	893	0.03%	0.004%
57	9.477	2621	2624	2625	rBV2	1249	755	0.03%	0.004%
58	9.731	2701	2703	2706	rVV3	908	686	0.03%	0.003%
59	9.764	2706	2713	2717	rVV6	1854	2244	0.08%	0.011%
60	9.915	2755	2760	2764	rBV6	1464	1777	0.06%	0.008%
61	9.934	2764	2766	2769	rVV4	887	675	0.02%	0.003%
62	10.059	2793	2805	2812	rVB5	5683	9199	0.34%	0.043%
63	10.149	2820	2833	2856	rBV	754205	1273881	46.57%	6.010%
64	10.310	2879	2883	2884	rVV5	2138	1245	0.05%	0.006%
65	10.320	2884	2886	2892	rVB7	2777	2257	0.08%	0.011%
66	10.362	2894	2899	2903	rBV6	2259	2736	0.10%	0.013%
67	10.445	2919	2925	2932	rVV7	2929	4321	0.16%	0.020%
68	10.481	2933	2936	2937	rVV3	2086	1324	0.05%	0.006%
69	10.513	2937	2946	2953	rVV3	6274	12662	0.46%	0.060%
70	10.542	2953	2955	2967	rVB10	3474	5738	0.21%	0.027%
71	10.625	2974	2981	2983	rBV6	1609	1728	0.06%	0.008%
72	10.673	2990	2996	2998	rBV6	1853	1819	0.07%	0.009%
73	10.715	3007	3009	3015	rBV7	879	797	0.03%	0.004%
74	10.754	3016	3021	3029	rBV9	4629	6669	0.24%	0.031%
75	10.834	3035	3046	3047	rBV5	8052	10683	0.39%	0.050%
76	10.850	3048	3051	3057	rVV3	10903	12114	0.44%	0.057%

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Instrument :
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 ClientSampleId :
 A4EJ6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
 Title : VOC Analysis

77	10.886	3060	3062	3071	rVB10	2974	3630	0.13%	0.017%
78	10.969	3078	3088	3093	rBV10	5956	11579	0.42%	0.055%
79	10.995	3093	3096	3097	rBV2	1994	1068	0.04%	0.005%
80	11.079	3112	3122	3131	rBV4	16761	29791	1.09%	0.141%
81	11.182	3142	3154	3172	rBV	1232882	1967916	71.94%	9.284%
82	11.323	3188	3198	3203	rBV4	17883	34944	1.28%	0.165%
83	11.471	3241	3244	3245	rBV3	2519	1624	0.06%	0.008%
84	11.506	3248	3255	3259	rVV9	5956	8825	0.32%	0.042%
85	11.554	3259	3270	3298	rVV	1433921	2293918	83.85%	10.822%
86	11.722	3312	3322	3335	rBV	17615	51933	1.90%	0.245%
87	11.863	3360	3366	3373	rBV9	7528	10468	0.38%	0.049%
88	12.034	3412	3419	3439	rVB3	28664	71825	2.63%	0.339%
89	12.117	3439	3445	3446	rBV5	5543	4877	0.18%	0.023%
90	12.317	3503	3507	3514	rVB6	6732	8563	0.31%	0.040%
91	12.464	3548	3553	3558	rBV5	10234	13764	0.50%	0.065%
92	12.535	3566	3575	3594	rVB4	95895	196257	7.17%	0.926%
93	12.657	3609	3613	3625	rVB10	16390	24061	0.88%	0.114%
94	12.728	3630	3635	3645	rVB8	14494	24400	0.89%	0.115%
95	13.352	3824	3829	3842	rVB8	18692	32979	1.21%	0.156%
96	13.580	3893	3900	3911	rVB2	78721	121569	4.44%	0.574%
97	14.587	4207	4213	4221	rBV2	42073	53783	1.97%	0.254%
98	15.355	4445	4452	4459	rBV4	30932	46097	1.69%	0.217%
99	15.516	4496	4502	4516	rVB6	44797	78360	2.86%	0.370%
100	16.387	4766	4773	4786	rVB3	29082	50291	1.84%	0.237%

Sum of corrected areas: 21197675

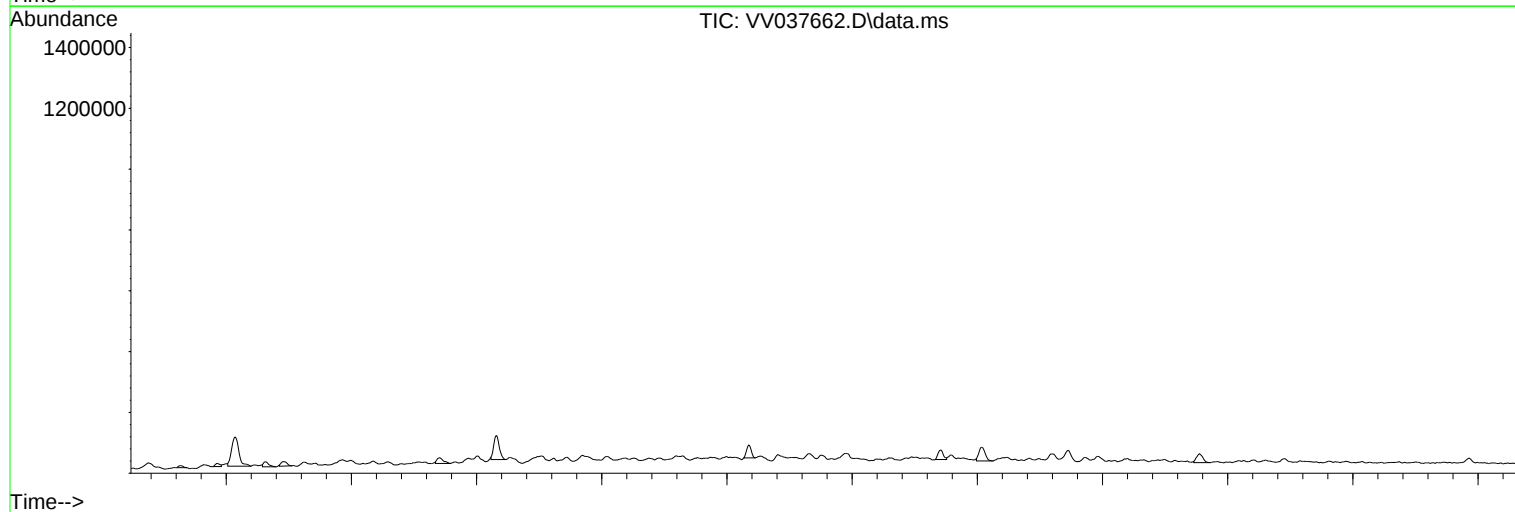
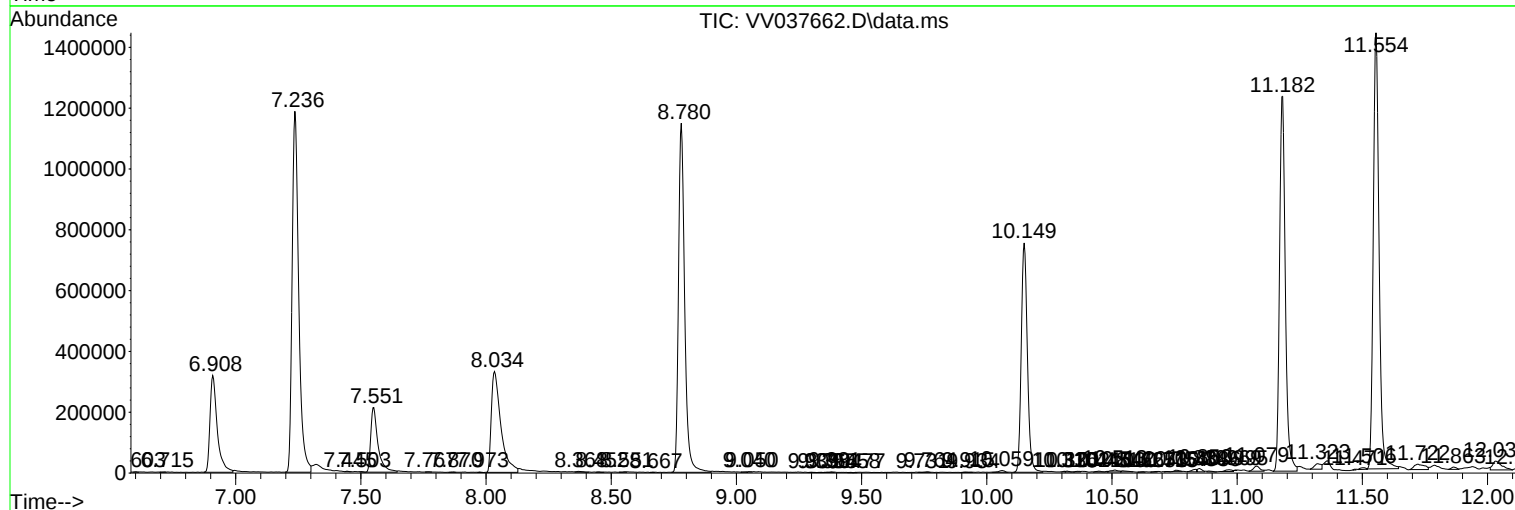
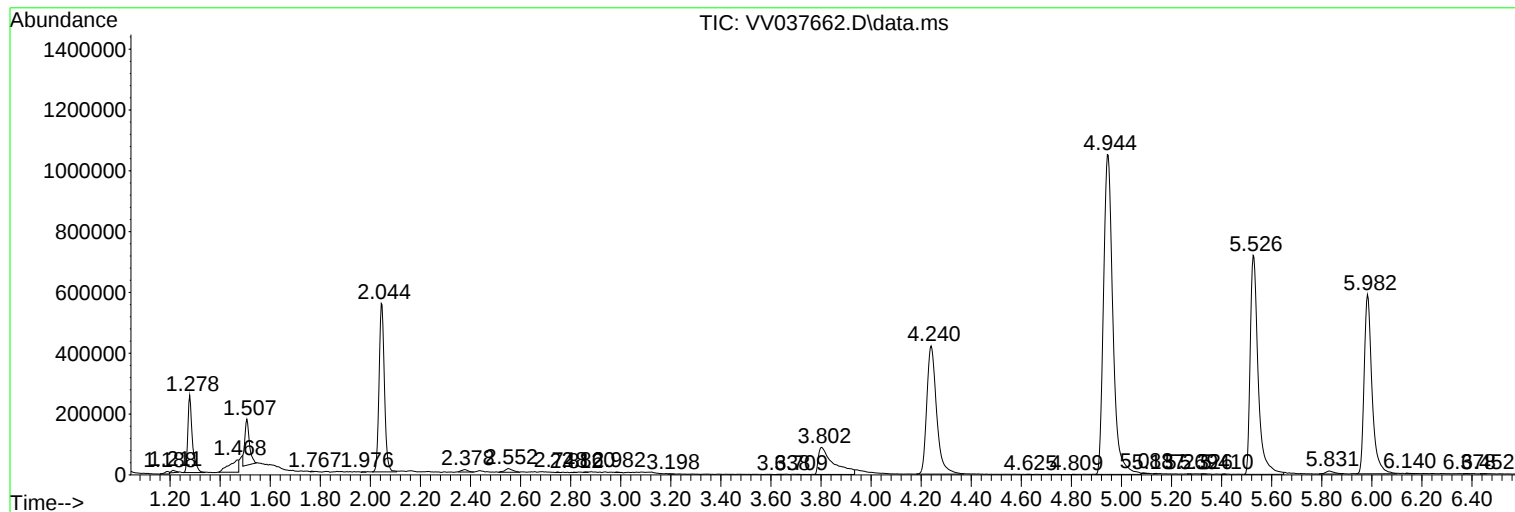
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4EJ6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
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A4EJ6ME

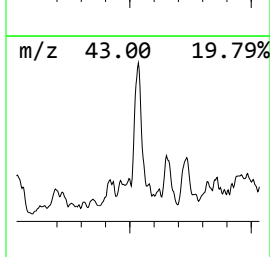
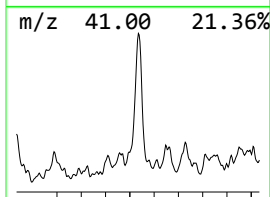
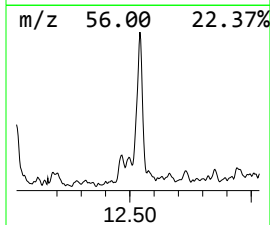
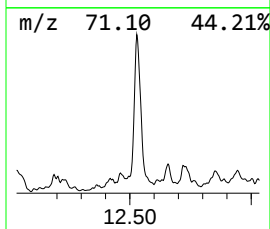
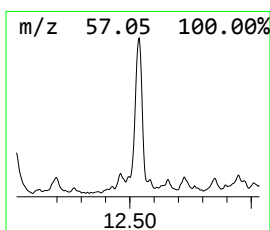
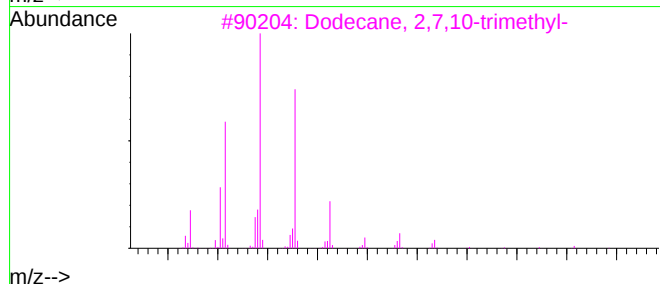
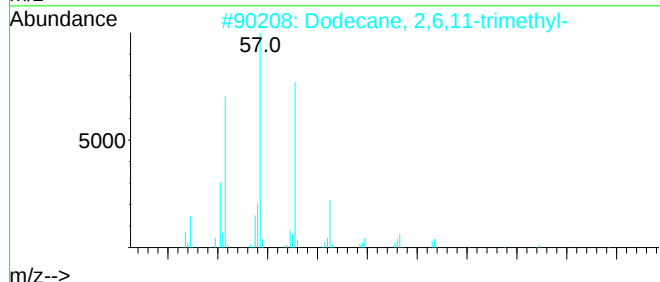
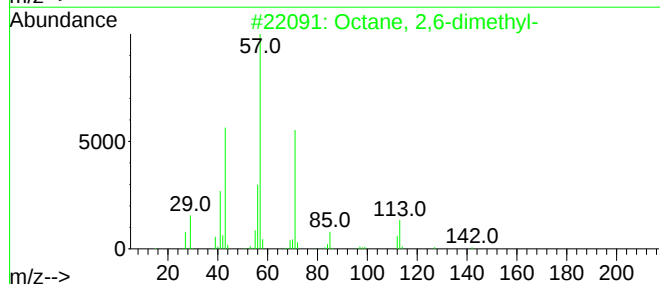
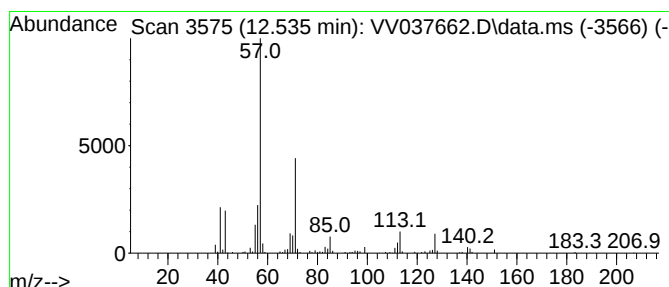
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.535	4.99 ug/L	196257	1,4-Dichlorobenzene-d4	11.182	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	70
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
5	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	59



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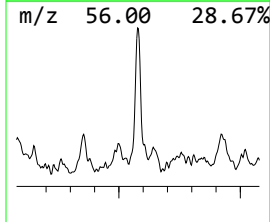
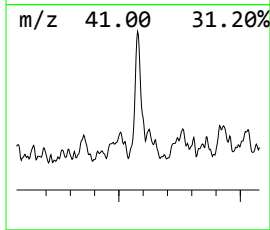
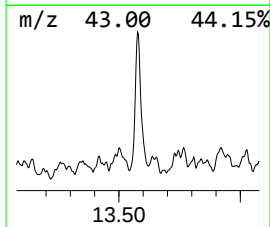
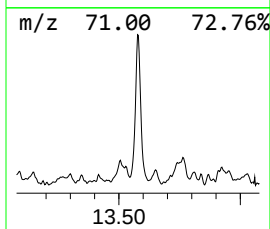
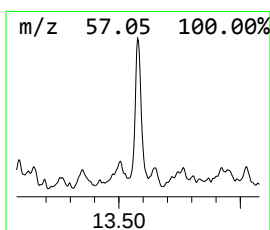
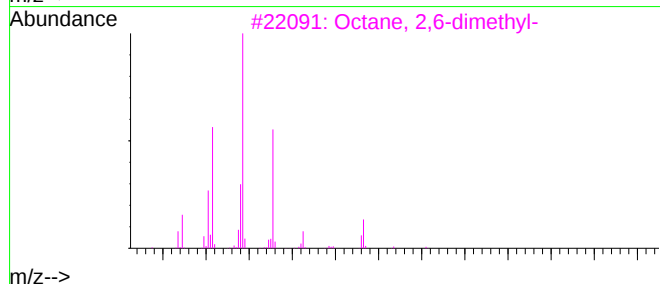
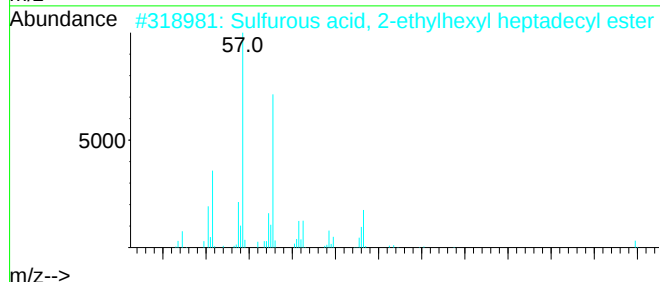
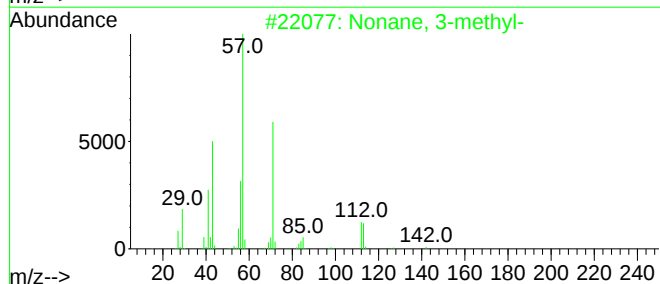
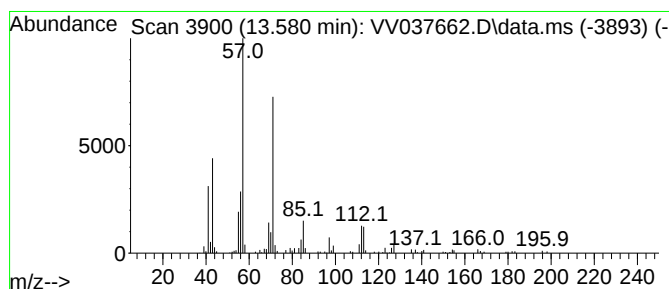
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.580	3.09 ug/L	121569	1,4-Dichlorobenzene-d4	11.182	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	80
2	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	74
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	72
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
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...	12.535	5.0	ug/L	196257	3	11.182	1967920	50.0
(DEL) Alkane: S...	13.580	3.1	ug/L	121569	3	11.182	1967920	50.0