

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071024\
 Data File : VW029505.D
 Acq On : 10 Jul 2024 14:38
 Operator : SY/MD
 Sample : P3177-11
 Misc : 5.35g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4BX4

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_W\Method\SFAMWLM070824SMA.M
 Title : SFAM01.0

Signal : TIC: VW029505.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.369	71	79	91	rBV	58135	151241	14.77%	2.115%
2	2.899	159	166	186	rVB	46750	135869	13.27%	1.900%
3	3.478	260	261	263	rBV2	618	456	0.04%	0.006%
4	3.539	265	271	274	rVV5	830	1443	0.14%	0.020%
5	3.716	298	300	302	rVV3	464	456	0.04%	0.006%
6	3.747	302	305	309	rVB5	808	1248	0.12%	0.017%
7	3.777	309	310	315	rVB3	476	611	0.06%	0.009%
8	3.820	315	317	320	rBV3	559	764	0.07%	0.011%
9	4.021	338	350	362	rBV	103745	347394	33.93%	4.858%
10	4.283	392	393	396	rVB2	429	349	0.03%	0.005%
11	4.338	399	402	403	rBV3	311	366	0.04%	0.005%
12	4.381	403	409	410	rBV3	2211	2887	0.28%	0.040%
13	4.588	440	443	445	rVB3	521	579	0.06%	0.008%
14	4.606	445	446	448	rBV2	599	508	0.05%	0.007%
15	4.783	473	475	480	rBV3	437	663	0.06%	0.009%
16	4.923	486	498	518	rBV2	17589	78564	7.67%	1.099%
17	5.149	529	535	537	rBV4	1132	2216	0.22%	0.031%
18	5.429	577	581	586	rVB4	1002	1715	0.17%	0.024%
19	5.478	586	589	593	rBV3	508	730	0.07%	0.010%
20	5.527	593	597	598	rBV2	446	635	0.06%	0.009%
21	5.655	615	618	619	rBV3	414	355	0.03%	0.005%
22	5.679	619	622	624	rVB2	526	452	0.04%	0.006%
23	5.716	624	628	631	rBV3	301	515	0.05%	0.007%
24	5.825	645	646	651	rVB2	532	715	0.07%	0.010%
25	5.935	657	664	665	rBV3	2724	4364	0.43%	0.061%
26	6.136	695	697	699	rBV2	407	401	0.04%	0.006%
27	6.155	699	700	706	rVB3	404	595	0.06%	0.008%
28	6.258	715	717	720	rBV2	288	441	0.04%	0.006%
29	6.289	720	722	725	rVB4	424	382	0.04%	0.005%
30	6.319	725	727	730	rVB2	350	349	0.03%	0.005%
31	6.478	750	753	756	rBV2	338	408	0.04%	0.006%
32	6.752	793	798	801	rVB3	408	582	0.06%	0.008%
33	6.825	809	810	814	rBV	300	407	0.04%	0.006%
34	6.929	819	827	829	rBV4	842	1964	0.19%	0.027%
35	7.075	841	851	862	rBV2	32025	98544	9.62%	1.378%
36	7.319	889	891	896	rBV5	472	714	0.07%	0.010%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
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37	7.551	927	929	931	rBV2	488	471	0.05%	0.007%
38	7.648	934	945	959	rBV	174436	421292	41.15%	5.891%
39	7.862	978	980	983	rVB2	387	380	0.04%	0.005%
40	7.984	998	1000	1004	rVB3	369	452	0.04%	0.006%
41	8.057	1008	1012	1014	rVB4	455	484	0.05%	0.007%
42	8.167	1027	1030	1032	rVB3	475	616	0.06%	0.009%
43	8.276	1037	1048	1069	rBV2	340184	1023854	100.00%	14.318%
44	8.691	1111	1116	1117	rVV4	796	1161	0.11%	0.016%
45	8.703	1117	1118	1119	rVV	1204	557	0.05%	0.008%
46	8.843	1131	1141	1157	rBV	447553	890156	86.94%	12.448%
47	9.038	1169	1173	1174	rBV4	1508	1668	0.16%	0.023%
48	9.270	1200	1211	1224	rBV	232912	487120	47.58%	6.812%
49	9.447	1237	1240	1242	rBV4	358	467	0.05%	0.007%
50	9.520	1250	1252	1256	rVB3	403	554	0.05%	0.008%
51	9.855	1306	1307	1309	rBV2	531	449	0.04%	0.006%
52	9.965	1322	1325	1328	rBV4	786	1048	0.10%	0.015%
53	10.032	1328	1336	1346	rBV	109880	204344	19.96%	2.858%
54	10.130	1348	1352	1358	rVB6	1384	3068	0.30%	0.043%
55	10.209	1364	1365	1368	rBV2	411	425	0.04%	0.006%
56	10.239	1368	1370	1373	rVB2	454	347	0.03%	0.005%
57	10.325	1375	1384	1392	rBV	382927	692996	67.69%	9.691%
58	10.520	1414	1416	1418	rVB3	446	350	0.03%	0.005%
59	10.575	1418	1425	1436	rBV	67848	123542	12.07%	1.728%
60	10.697	1439	1445	1452	rVB2	5688	9528	0.93%	0.133%
61	10.770	1454	1457	1460	rVB4	363	446	0.04%	0.006%
62	10.837	1462	1468	1470	rBV5	1273	2395	0.23%	0.033%
63	10.922	1475	1482	1499	rBV	115579	210359	20.55%	2.942%
64	11.178	1520	1524	1528	rVV6	991	1385	0.14%	0.019%
65	11.239	1532	1534	1537	rVB3	409	373	0.04%	0.005%
66	11.331	1548	1549	1552	rBV3	384	345	0.03%	0.005%
67	11.398	1557	1560	1567	rBV6	1547	2059	0.20%	0.029%
68	11.507	1575	1578	1580	rBV2	575	542	0.05%	0.008%
69	11.629	1588	1598	1607	rVV	532136	873853	85.35%	12.220%
70	11.812	1625	1628	1629	rBV2	483	472	0.05%	0.007%
71	11.831	1629	1631	1636	rVV4	1020	1823	0.18%	0.025%
72	11.922	1643	1646	1647	rBV3	489	420	0.04%	0.006%
73	12.013	1659	1661	1665	rVB3	516	715	0.07%	0.010%
74	12.068	1665	1670	1673	rBV5	885	1466	0.14%	0.021%
75	12.117	1673	1678	1679	rBV4	539	770	0.08%	0.011%
76	12.135	1679	1681	1682	rVV3	585	467	0.05%	0.007%

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Integration Parameters: LSCINT.P

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77	12.160	1682	1685	1692	rVV7	1363	2712	0.26%	0.038%
78	12.251	1695	1700	1703	rVB4	1388	2492	0.24%	0.035%
79	12.300	1703	1708	1709	rVB3	374	457	0.04%	0.006%
80	12.324	1709	1712	1713	rBV2	1010	1181	0.12%	0.017%
81	12.410	1723	1726	1727	rBV3	591	624	0.06%	0.009%
82	12.434	1728	1730	1733	rVV3	391	519	0.05%	0.007%
83	12.599	1750	1757	1764	rVB2	18246	35642	3.48%	0.498%
84	12.690	1764	1772	1778	rBV	144412	239604	23.40%	3.351%
85	12.769	1779	1785	1792	rVB7	4299	12455	1.22%	0.174%
86	12.855	1795	1799	1800	rBV4	1020	1140	0.11%	0.016%
87	12.958	1807	1816	1821	rBV8	5144	12267	1.20%	0.172%
88	13.074	1831	1835	1839	rBV4	2257	2878	0.28%	0.040%
89	13.123	1840	1843	1844	rBV3	1313	1354	0.13%	0.019%
90	13.190	1845	1854	1860	rVB	19352	39055	3.81%	0.546%
91	13.294	1867	1871	1876	rVB2	8272	12610	1.23%	0.176%
92	13.403	1881	1889	1897	rBV2	28368	55877	5.46%	0.781%
93	13.556	1908	1914	1919	rBV	314197	517213	50.52%	7.233%
94	13.763	1943	1948	1955	rVB3	13555	24816	2.42%	0.347%
95	13.848	1956	1962	1968	rBV	174240	288701	28.20%	4.037%
96	14.062	1993	1997	2002	rBV2	11670	19369	1.89%	0.271%
97	14.178	2014	2016	2021	rVB5	2231	3273	0.32%	0.046%
98	14.318	2035	2039	2045	rBV5	7451	14155	1.38%	0.198%
99	14.495	2063	2068	2079	rBV7	9439	33127	3.24%	0.463%
100	15.318	2200	2203	2209	rVB2	14885	26302	2.57%	0.368%

Sum of corrected areas: 7150924

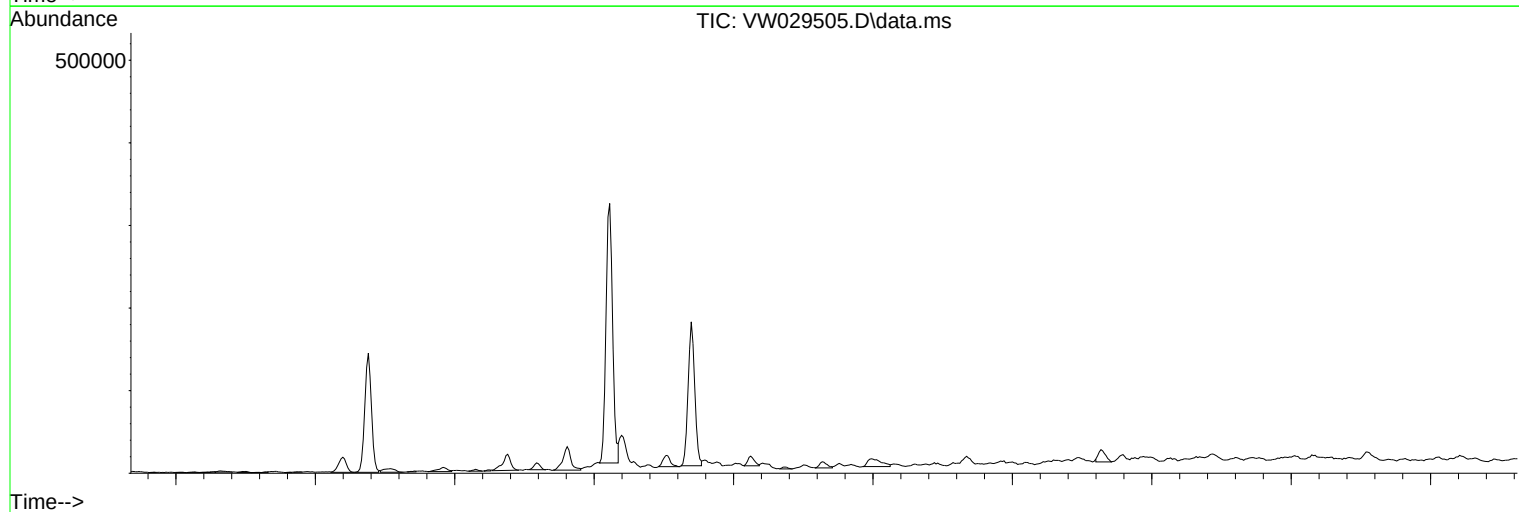
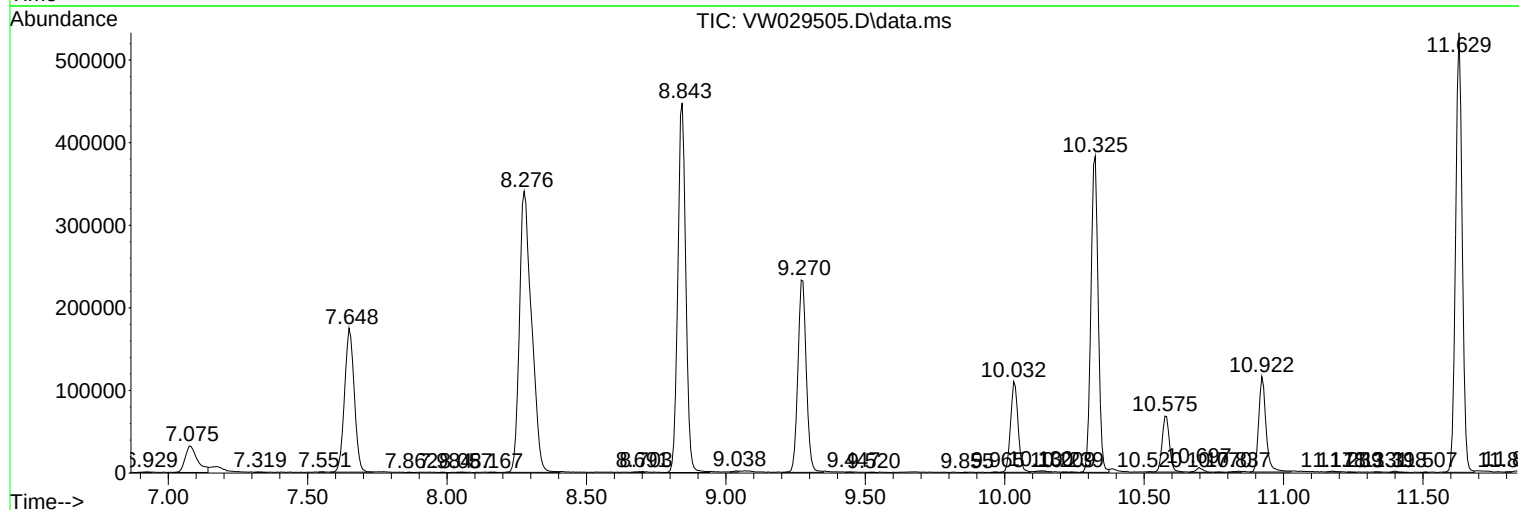
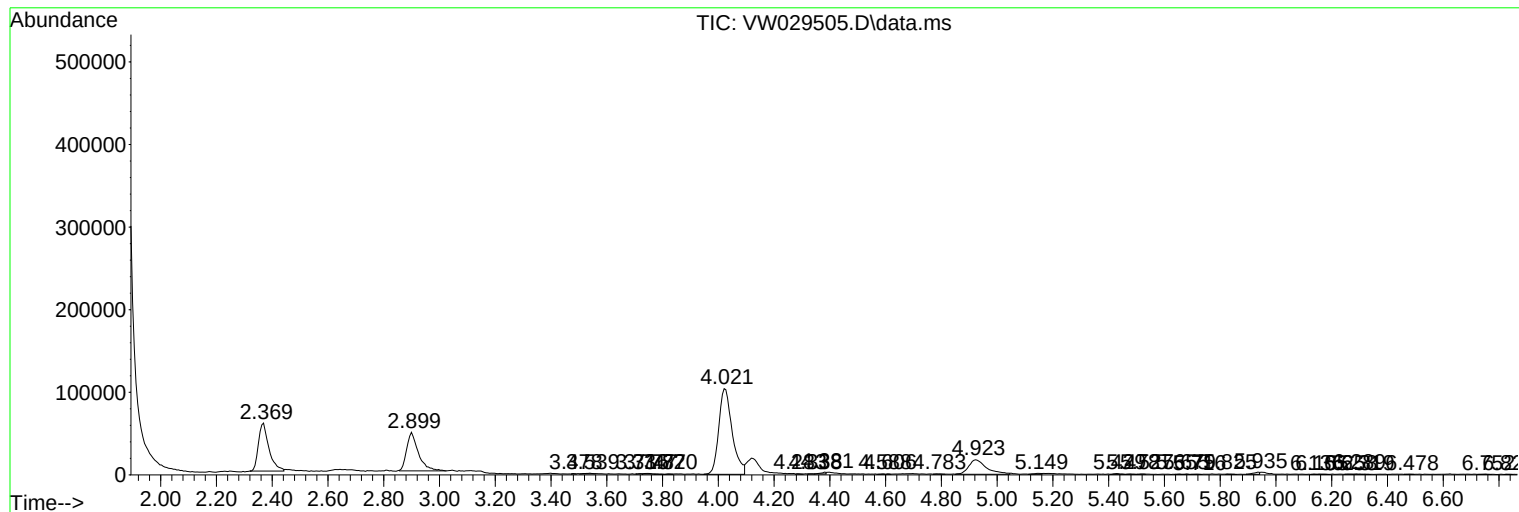
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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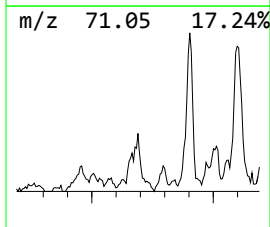
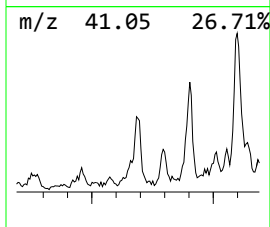
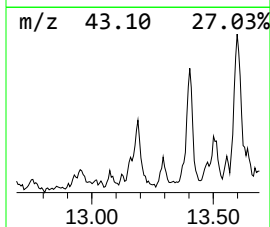
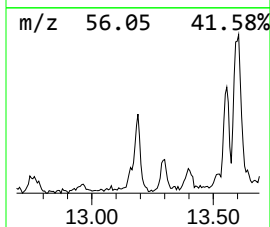
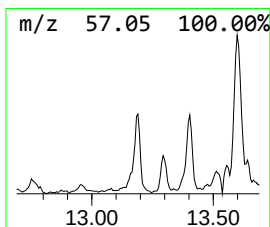
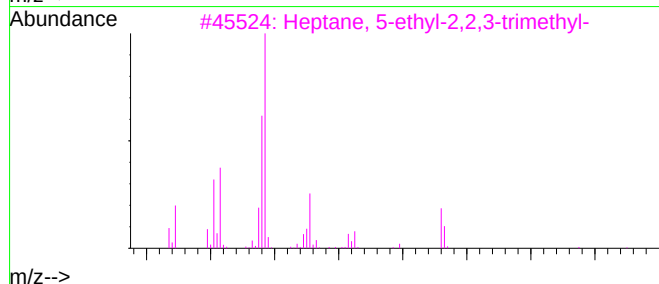
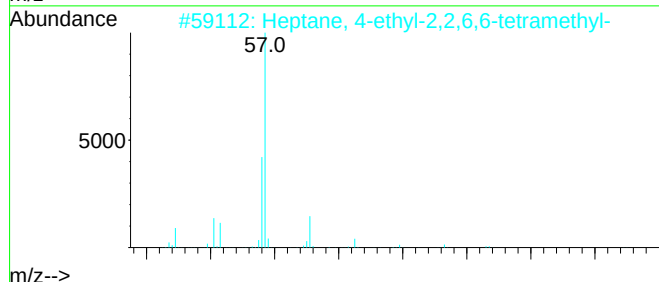
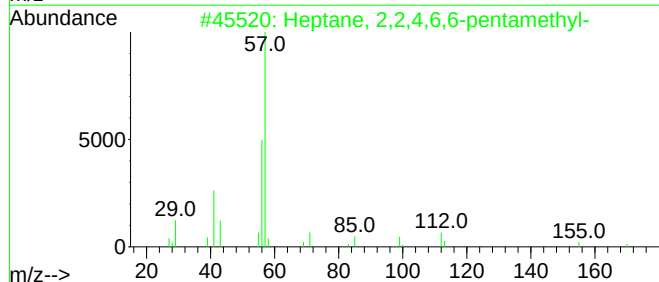
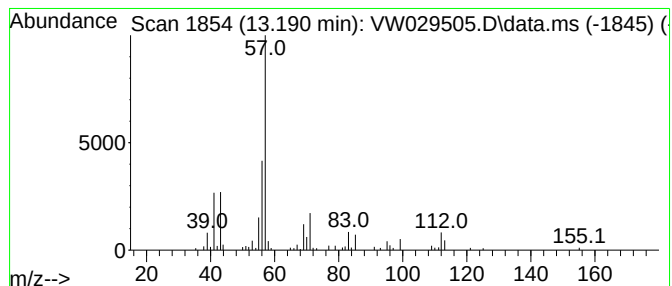
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	1.89 ug/L	39055	1,4-Dichlorobenzene-d4	13.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
2	Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	59
3	Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	53
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53
5	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	53



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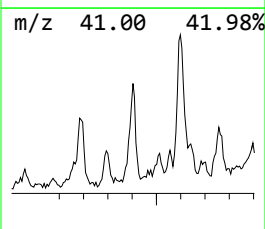
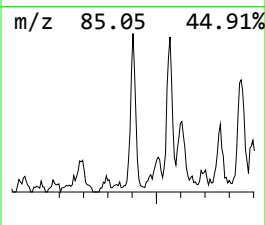
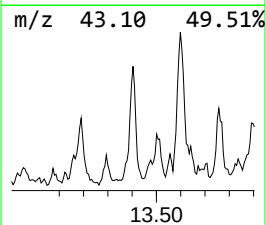
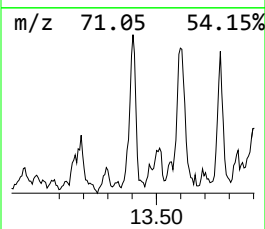
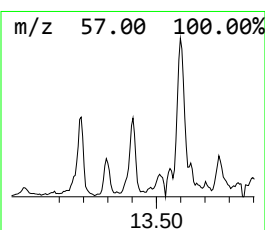
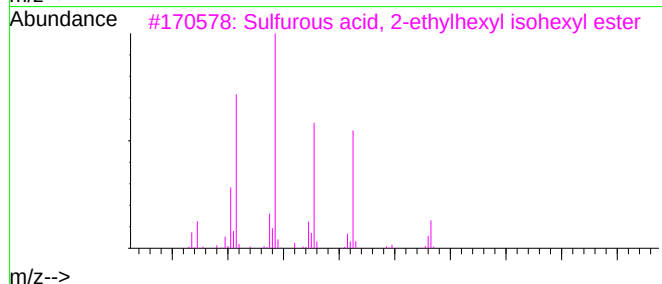
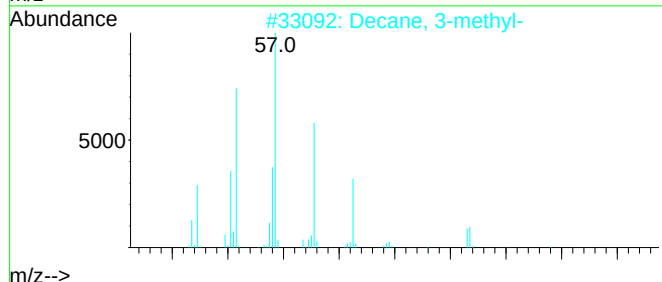
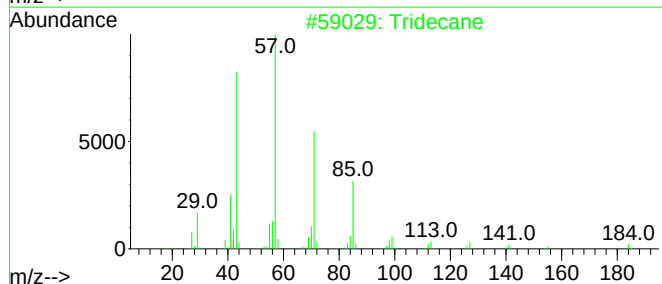
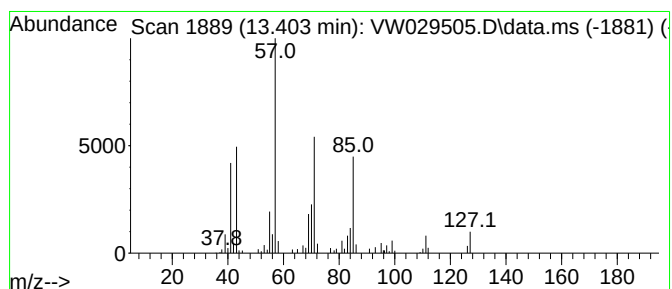
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.403	2.70 ug/L	55877	1,4-Dichlorobenzene-d4	13.556	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	59
2	Decane, 3-methyl-	156	C11H24	013151-34-3	59
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	50
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	50
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50



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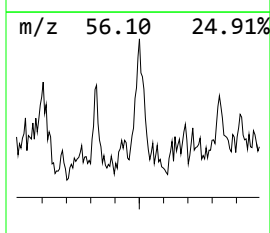
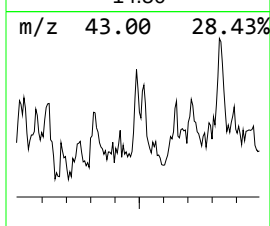
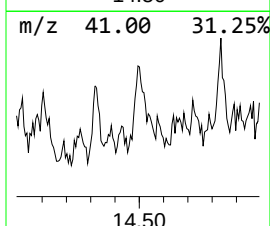
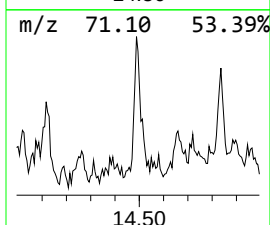
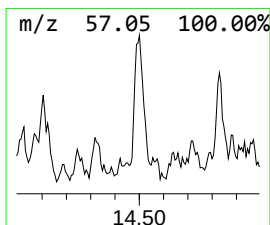
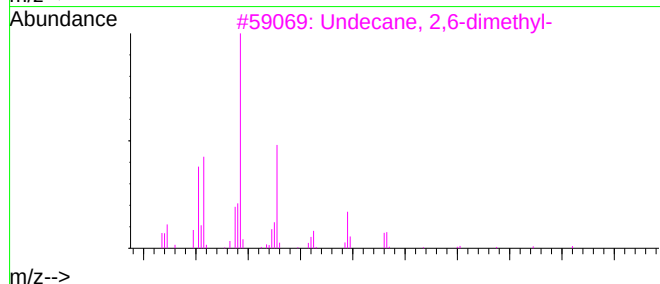
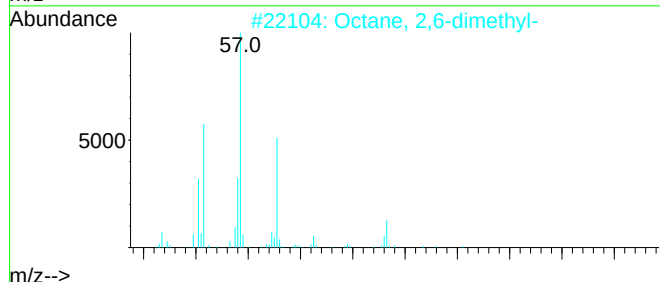
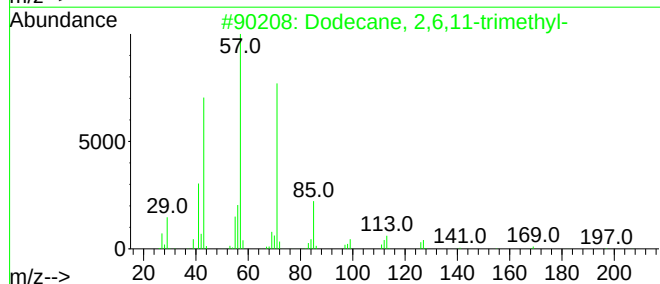
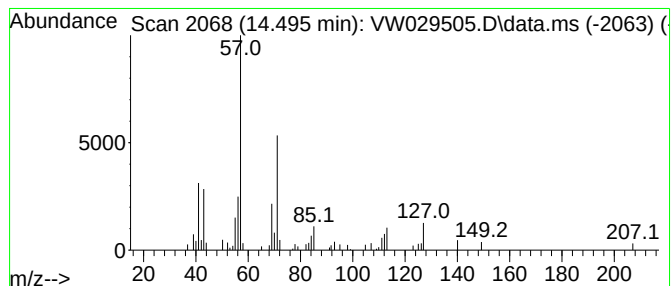
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.495	1.60 ug/L	33127	1,4-Dichlorobenzene-d4	13.556	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	59
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071024\
Data File : VW029505.D
Acq On : 10 Jul 2024 14:38
Operator : SY/MD
Sample : P3177-11
Misc : 5.35g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4BX4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

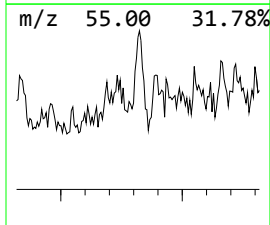
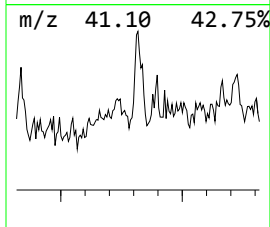
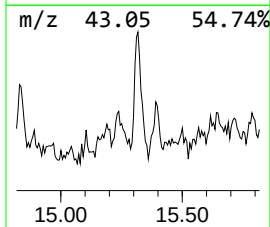
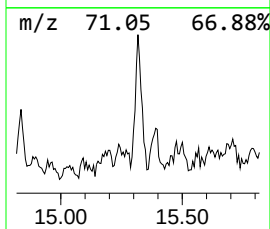
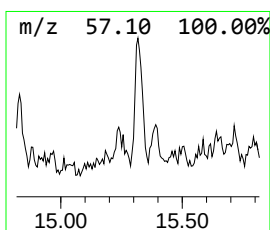
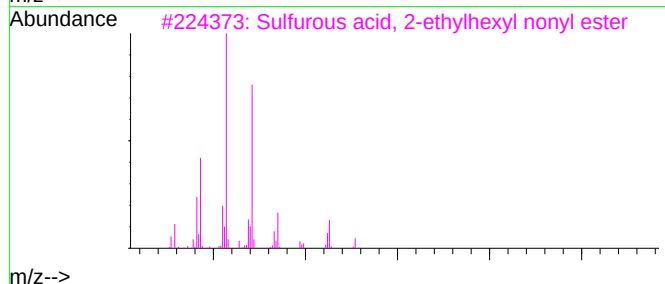
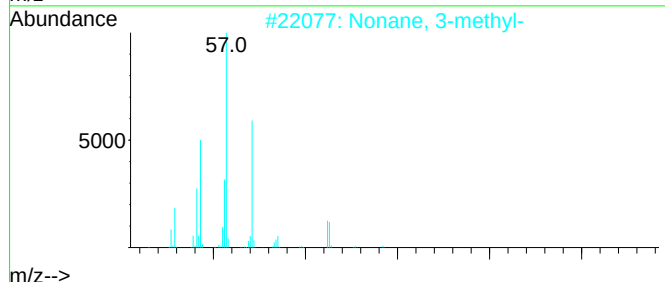
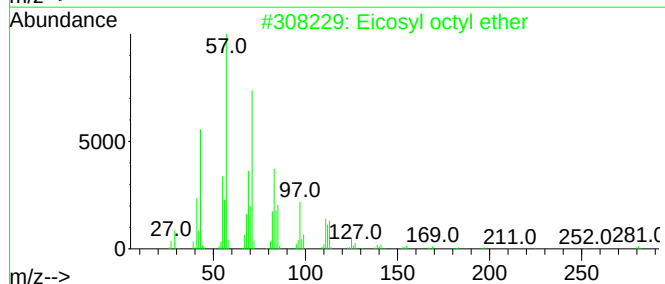
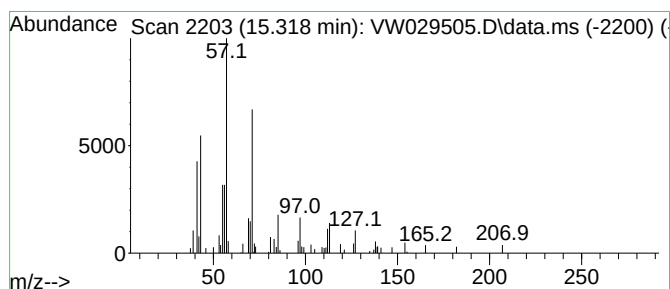
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosyl octyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	1.27 ug/L	26302	1,4-Dichlorobenzene-d4	13.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl octyl ether	410	C28H58O	1000406-38-8	64
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	59
3	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	58
4	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	53
5	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071024\
Data File : VW029505.D
Acq On : 10 Jul 2024 14:38
Operator : SY/MD
Sample : P3177-11
Misc : 5.35g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4BX4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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...	13.190	1.9	ug/L	39055	3	13.556	517213	25.0
(DEL) Alkane: S...	13.403	2.7	ug/L	55877	3	13.556	517213	25.0
(DEL) Alkane: S...	14.495	1.6	ug/L	33127	3	13.556	517213	25.0
Eicosyl octyl e...	15.318	1.3	ug/L	26302	3	13.556	517213	25.0