

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042416.D
 Acq On : 19 Jul 2024 20:48
 Operator : JC/MD
 Sample : P3238-19ME
 Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CH4ME

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_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042416.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	27	rBV	30766	37743	5.72%	0.551%
2	1.374	43	47	48	rBV	20768	25839	3.92%	0.377%
3	2.276	189	195	211	rBV	96573	185895	28.17%	2.713%
4	2.721	261	268	274	rBV	10658	22501	3.41%	0.328%
5	2.941	298	304	320	rVB	7798	22013	3.34%	0.321%
6	4.495	551	559	575	rBV	31133	114310	17.33%	1.668%
7	5.056	639	651	671	rBV	74515	232893	35.30%	3.399%
8	5.830	769	778	787	rVB5	1927	5400	0.82%	0.079%
9	5.958	787	799	817	rBV2	220728	622267	94.31%	9.081%
10	6.757	921	930	947	rBV	225535	542948	82.29%	7.924%
11	7.233	1001	1008	1012	rBV3	2724	5986	0.91%	0.087%
12	7.306	1012	1020	1027	rBV	120460	270061	40.93%	3.941%
13	7.550	1055	1060	1067	rVV3	3384	6510	0.99%	0.095%
14	7.763	1087	1095	1102	rVV2	7799	16341	2.48%	0.238%
15	7.952	1118	1126	1135	rBV6	8208	18278	2.77%	0.267%
16	8.184	1157	1164	1167	rBV	4137	7977	1.21%	0.116%
17	8.269	1174	1178	1181	rBV2	4799	6791	1.03%	0.099%
18	8.324	1181	1187	1194	rBV	69488	116951	17.73%	1.707%
19	8.434	1200	1205	1208	rBV2	6344	11553	1.75%	0.169%
20	8.598	1225	1232	1235	rBV	27868	54324	8.23%	0.793%
21	8.647	1235	1240	1248	rVV	327908	533858	80.91%	7.791%
22	8.720	1248	1252	1256	rVV	18321	30209	4.58%	0.441%
23	8.769	1256	1260	1267	rVB	20164	33735	5.11%	0.492%
24	8.842	1267	1272	1278	rVB3	4589	7784	1.18%	0.114%
25	8.909	1278	1283	1286	rBV2	4991	7706	1.17%	0.112%
26	8.952	1286	1290	1302	rVB2	50019	124234	18.83%	1.813%
27	9.098	1307	1314	1320	rVB	15300	24857	3.77%	0.363%
28	9.153	1320	1323	1327	rBV3	2693	4428	0.67%	0.065%
29	9.226	1332	1335	1339	rVB	5887	7260	1.10%	0.106%
30	9.287	1339	1345	1351	rVB5	9549	17812	2.70%	0.260%
31	9.391	1351	1362	1374	rBV2	137590	310425	47.05%	4.530%
32	9.500	1375	1380	1385	rBV3	27610	49233	7.46%	0.718%
33	9.561	1385	1390	1394	rVB2	18389	27994	4.24%	0.409%
34	9.616	1394	1399	1403	rBV	52465	78424	11.89%	1.144%
35	9.696	1409	1412	1417	rVB5	4809	7006	1.06%	0.102%
36	9.756	1417	1422	1426	rVB2	5490	7505	1.14%	0.110%

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 ALS Vial : 14 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 A4CH4ME

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_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

37	9.830	1426	1434	1437	rBV3	24167	47638	7.22%	0.695%
38	9.860	1437	1439	1442	rVV3	9679	13458	2.04%	0.196%
39	9.897	1442	1445	1451	rVB	29403	43530	6.60%	0.635%
40	10.006	1456	1463	1466	rBV	30677	43612	6.61%	0.636%
41	10.055	1466	1471	1486	rVB	457611	651848	98.80%	9.513%
42	10.177	1486	1491	1498	rVB5	8846	16878	2.56%	0.246%
43	10.275	1502	1507	1509	rBV2	14642	20881	3.16%	0.305%
44	10.360	1517	1521	1531	rVB3	22611	39628	6.01%	0.578%
45	10.451	1531	1536	1542	rBV2	11227	15967	2.42%	0.233%
46	10.531	1545	1549	1551	rBV2	6801	9005	1.36%	0.131%
47	10.586	1551	1558	1565	rVB4	32646	58491	8.87%	0.854%
48	10.671	1565	1572	1577	rBV3	15191	30299	4.59%	0.442%
49	10.781	1582	1590	1594	rVV2	34457	57746	8.75%	0.843%
50	10.829	1594	1598	1599	rVV2	9741	13689	2.07%	0.200%
51	10.854	1599	1602	1605	rVV3	23066	34755	5.27%	0.507%
52	10.897	1605	1609	1613	rVV2	24518	38946	5.90%	0.568%
53	10.945	1613	1617	1622	rVB4	7230	11926	1.81%	0.174%
54	11.031	1627	1631	1634	rVB2	16277	20238	3.07%	0.295%
55	11.086	1634	1640	1642	rBV3	15271	21950	3.33%	0.320%
56	11.195	1650	1658	1666	rBV	247973	367101	55.64%	5.357%
57	11.335	1678	1681	1685	rBV4	4060	5995	0.91%	0.087%
58	11.384	1686	1689	1693	rVV3	4779	6745	1.02%	0.098%
59	11.427	1693	1696	1700	rVV	12474	17488	2.65%	0.255%
60	11.476	1700	1704	1709	rVB2	41418	50577	7.67%	0.738%
61	11.634	1726	1730	1734	rVB5	7480	9589	1.45%	0.140%
62	11.683	1735	1738	1740	rVV3	6092	6223	0.94%	0.091%
63	11.713	1740	1743	1746	rVB	14278	14340	2.17%	0.209%
64	11.750	1746	1749	1752	rBV3	3597	5227	0.79%	0.076%
65	11.841	1760	1764	1766	rBV3	5166	7895	1.20%	0.115%
66	11.939	1776	1780	1783	rBV3	9536	12510	1.90%	0.183%
67	11.976	1783	1786	1788	rVV4	4151	5842	0.89%	0.085%
68	12.024	1788	1794	1800	rVV	507255	659792	100.00%	9.629%
69	12.073	1800	1802	1804	rVV	8309	8768	1.33%	0.128%
70	12.104	1804	1807	1810	rVB3	8564	10490	1.59%	0.153%
71	12.317	1837	1842	1850	rBV	362885	491246	74.45%	7.169%
72	12.421	1855	1859	1864	rBV	32682	38099	5.77%	0.556%
73	12.463	1864	1866	1872	rVB5	4743	8137	1.23%	0.119%
74	12.555	1875	1881	1883	rBV6	3572	6623	1.00%	0.097%
75	12.683	1898	1902	1906	rBV4	3286	4286	0.65%	0.063%
76	12.768	1912	1916	1921	rBV7	1889	3809	0.58%	0.056%

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 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CH4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

77	12.817	1921	1924	1928	rVB4	3247	4012	0.61%	0.059%
78	12.884	1928	1935	1942	rBV7	6765	17460	2.65%	0.255%
79	12.975	1947	1950	1955	rVB4	4587	6028	0.91%	0.088%
80	13.042	1958	1961	1965	rVB3	3390	4155	0.63%	0.061%
81	13.268	1994	1998	2001	rBV	13449	17507	2.65%	0.255%
82	13.384	2013	2017	2018	rBV2	3874	4021	0.61%	0.059%
83	13.512	2033	2038	2045	rVB	19528	28521	4.32%	0.416%
84	13.695	2063	2068	2071	rBV5	2217	4494	0.68%	0.066%
85	13.774	2077	2081	2089	rVV	20432	30700	4.65%	0.448%
86	14.036	2120	2124	2129	rVB2	6049	7514	1.14%	0.110%
87	14.640	2219	2223	2230	rVB	12472	18032	2.73%	0.263%
88	14.780	2243	2246	2249	rVV	11358	15612	2.37%	0.228%
89	14.817	2249	2252	2256	rVV2	14771	18503	2.80%	0.270%
90	14.932	2267	2271	2278	rVB2	14483	20555	3.12%	0.300%
91	15.048	2284	2290	2296	rBV2	32613	46080	6.98%	0.672%
92	15.213	2313	2317	2323	rVV3	3454	5952	0.90%	0.087%
93	15.377	2339	2344	2349	rBV6	2237	5014	0.76%	0.073%
94	15.481	2357	2361	2367	rBV3	7126	14739	2.23%	0.215%
95	15.615	2378	2383	2386	rBV2	6952	10647	1.61%	0.155%
96	15.652	2386	2389	2395	rVB2	4838	7756	1.18%	0.113%
97	15.737	2397	2403	2408	rVB6	6680	12598	1.91%	0.184%
98	15.981	2441	2443	2451	rVB7	2609	4616	0.70%	0.067%
99	16.097	2456	2462	2469	rVB7	3432	7250	1.10%	0.106%
100	16.328	2494	2500	2506	rBV3	5590	10195	1.55%	0.149%

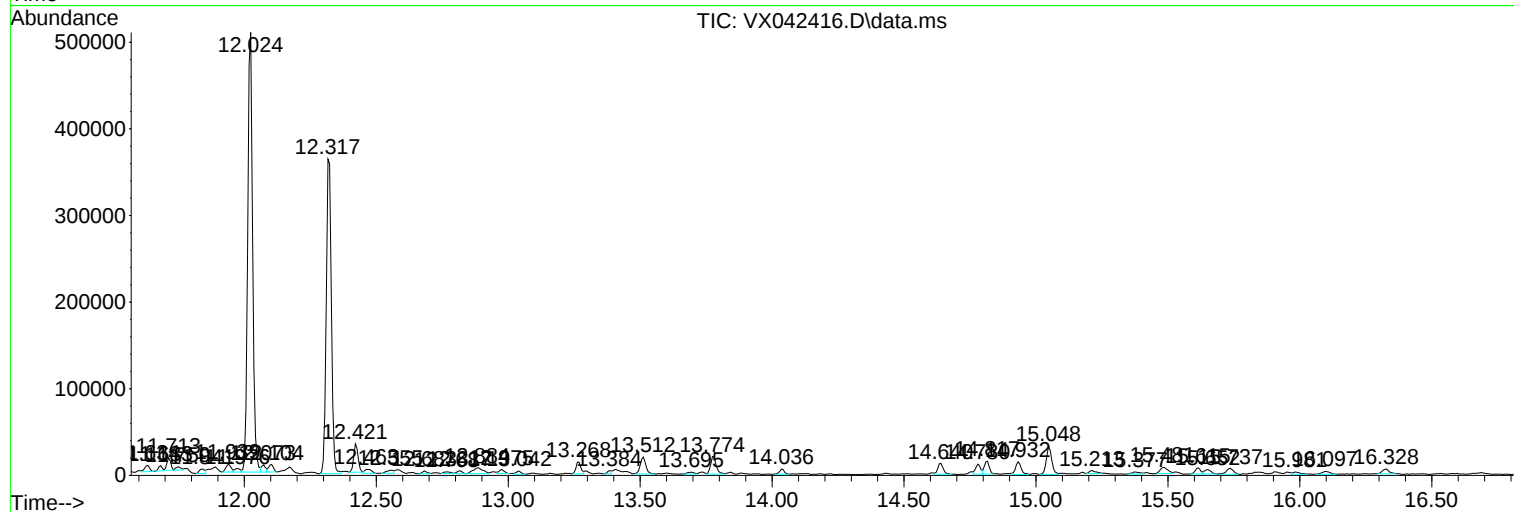
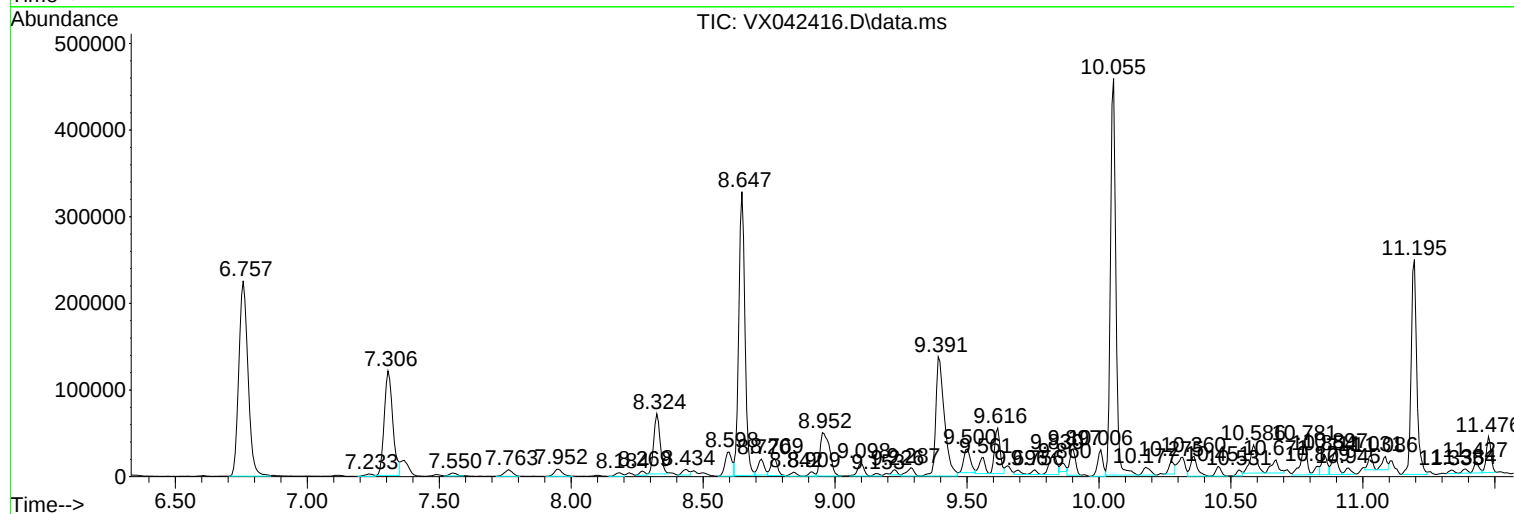
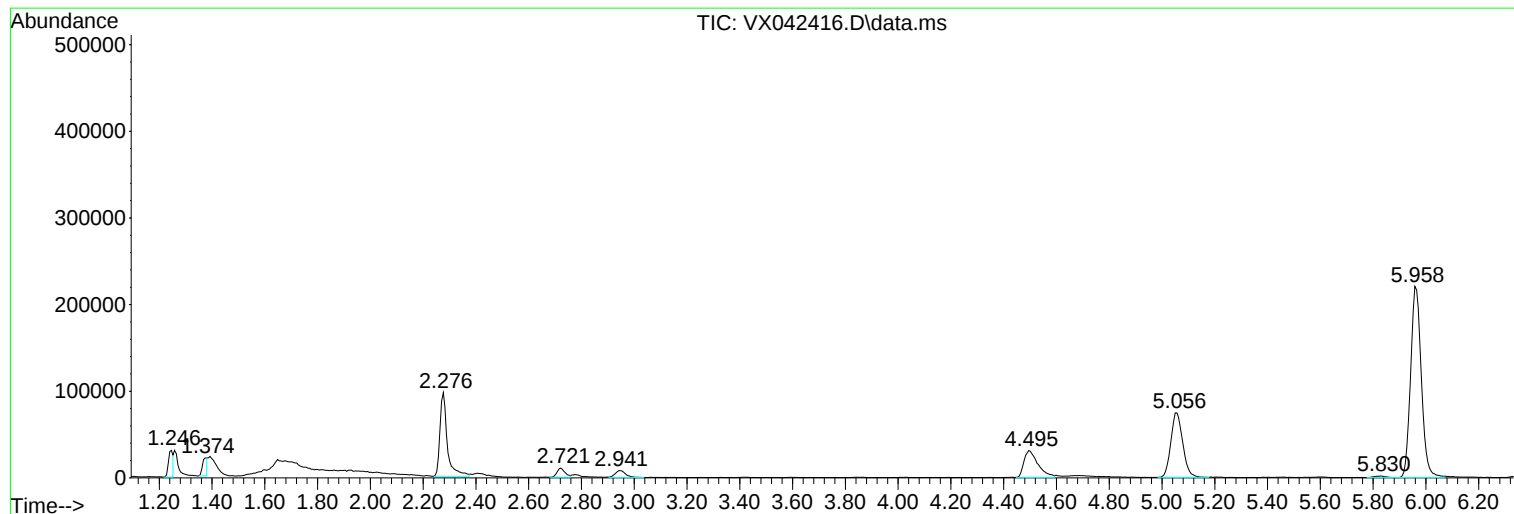
Sum of corrected areas: 6852279

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

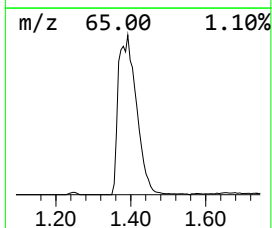
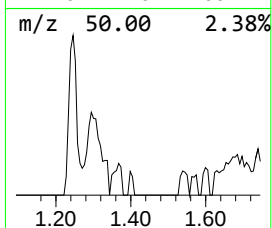
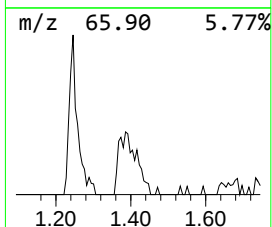
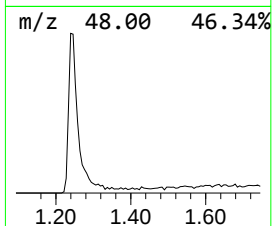
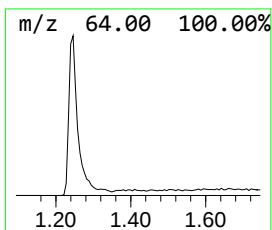
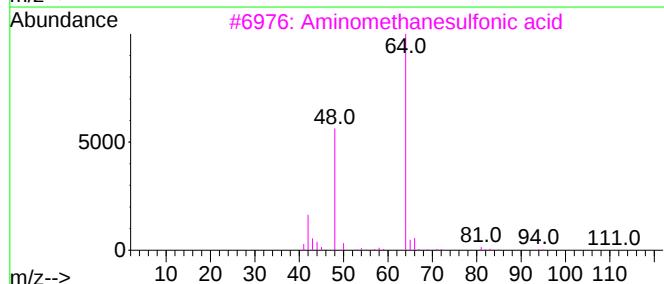
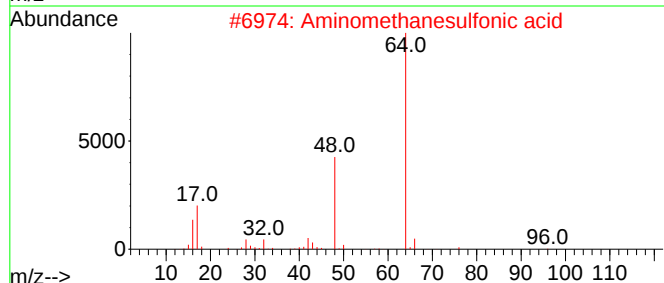
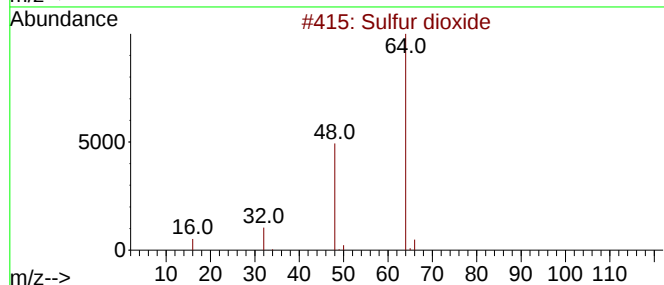
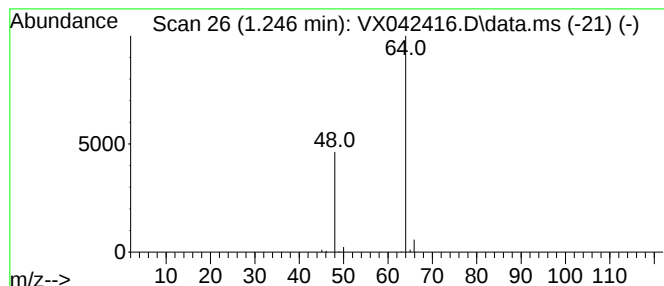
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	3.48 ug/L	37743	1,4-Difluorobenzene	6.757

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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Instrument :
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A4CH4ME

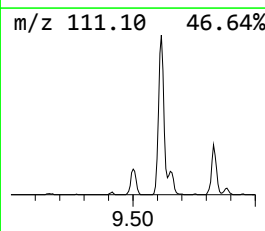
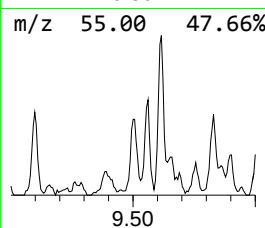
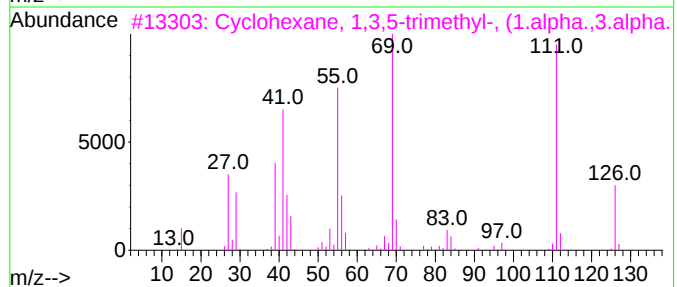
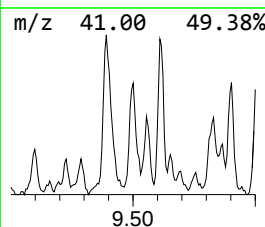
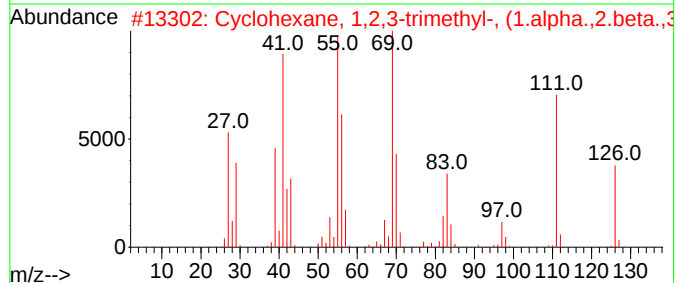
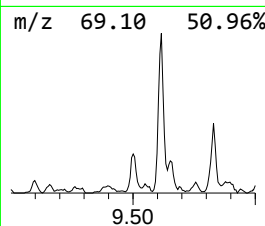
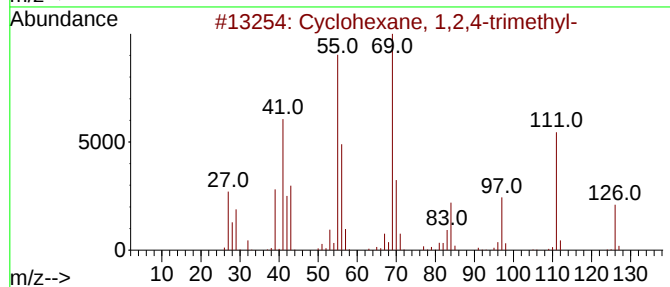
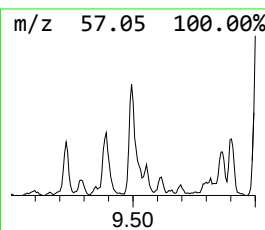
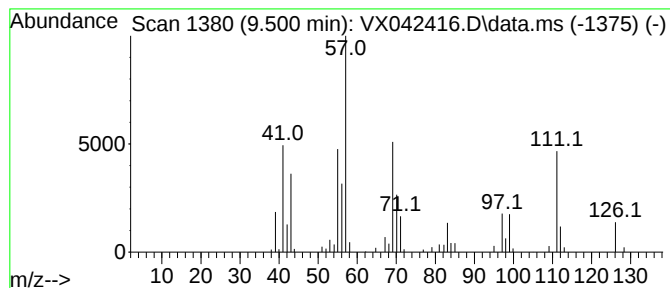
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic9.500 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.500	3.78 ug/L	49233	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	43
2			Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001678-81-5	38
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	38
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	38
5			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	35



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

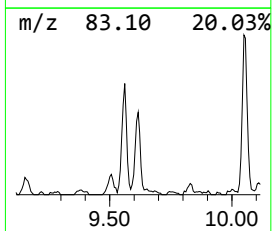
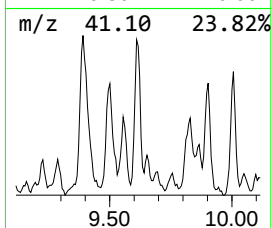
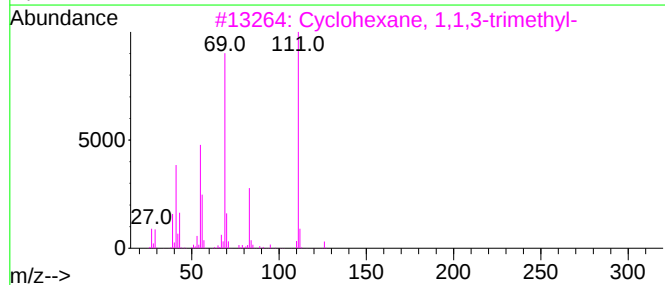
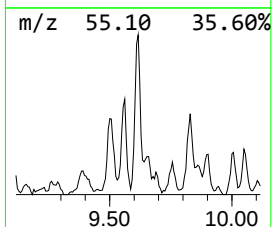
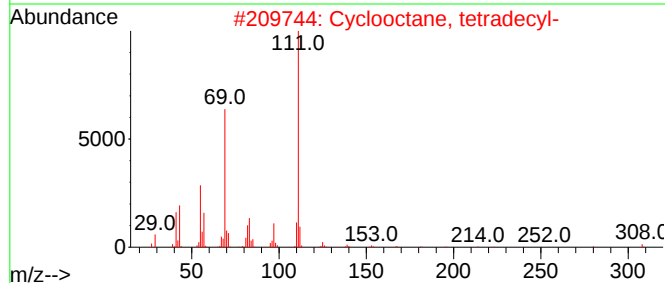
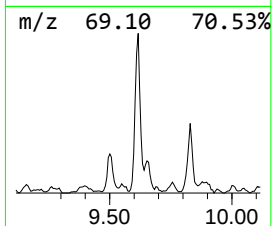
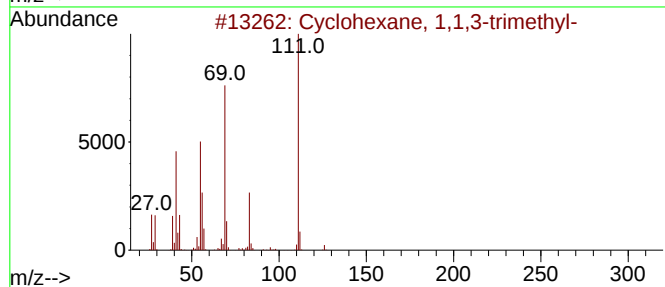
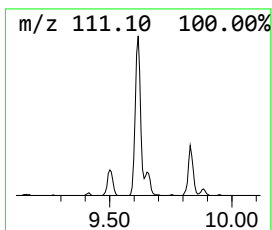
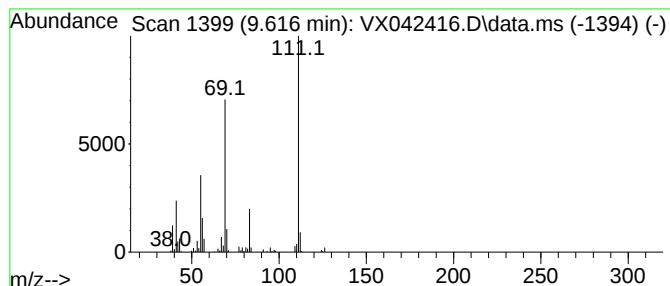
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic9.616 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	6.02 ug/L	78424	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	74
2			Cyclooctane, tetradecyl-	308	C22H44	149003-36-1	72
3			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	70
4			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	64
5			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

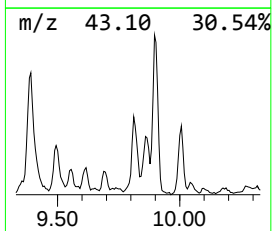
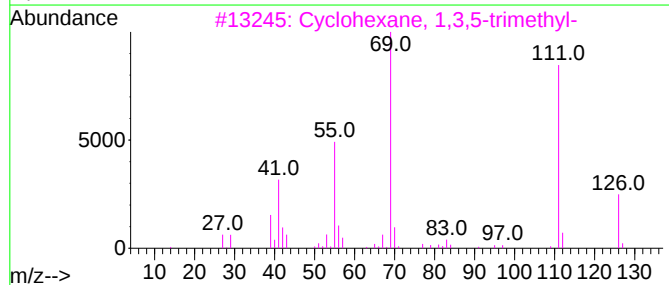
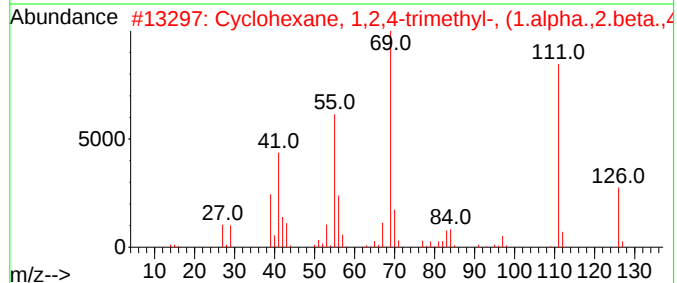
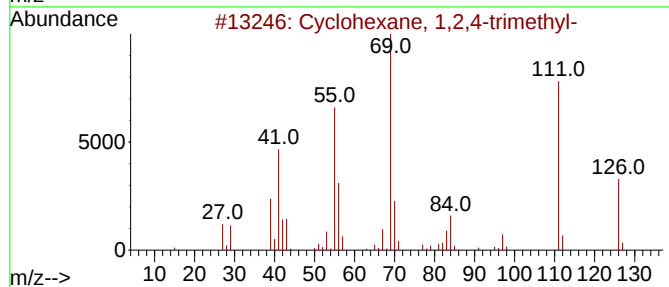
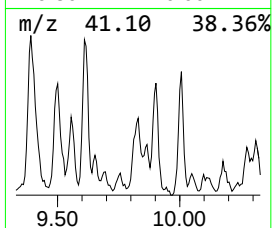
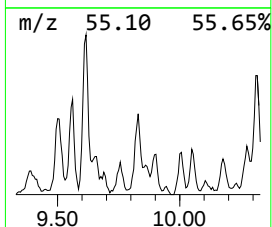
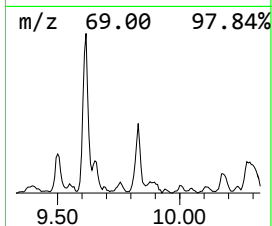
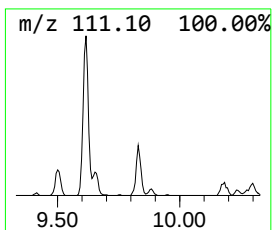
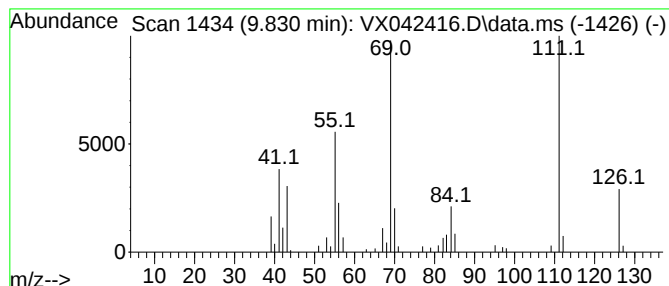
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic9.830 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.830	3.65 ug/L	47638	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	94
2			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	90
3			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	87
4			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
5			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

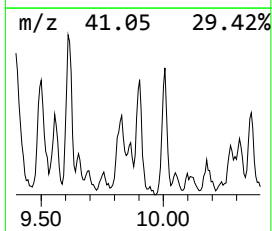
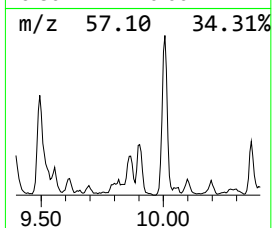
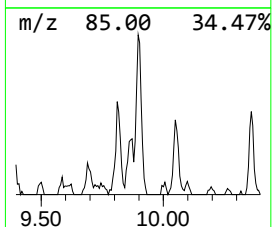
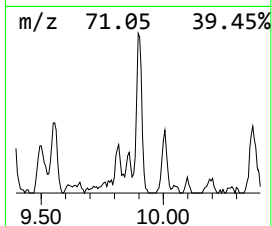
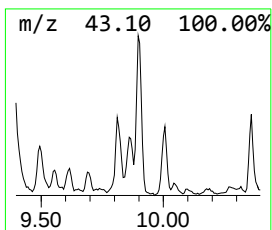
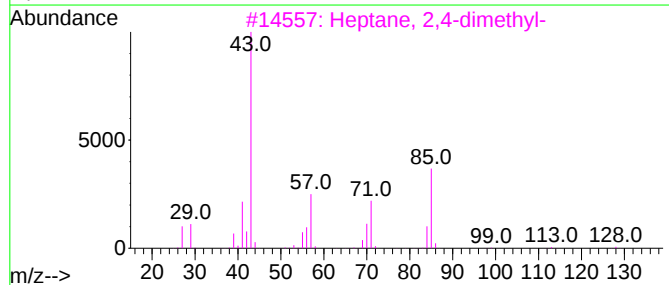
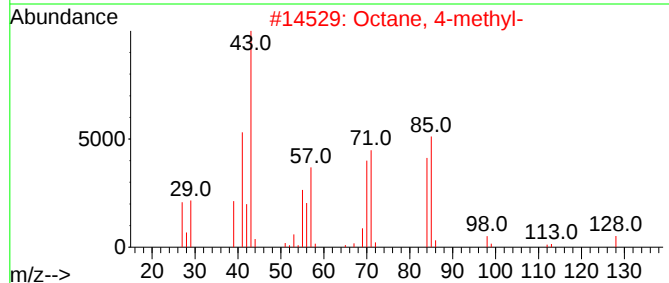
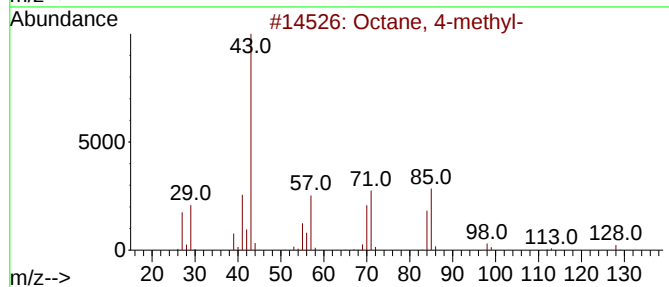
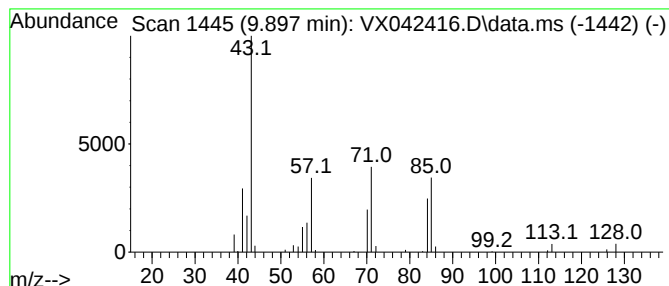
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.897	3.34 ug/L	43530	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	72
2			Octane, 4-methyl-	128	C9H20	002216-34-4	64
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
5			Undecane, 5-methyl-	170	C12H26	001632-70-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

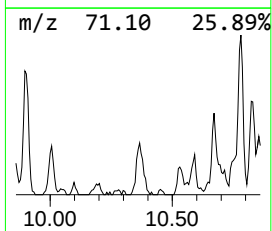
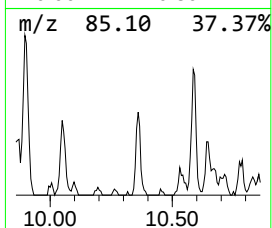
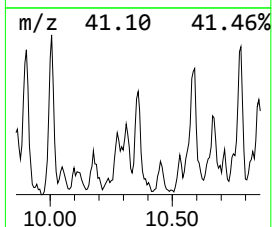
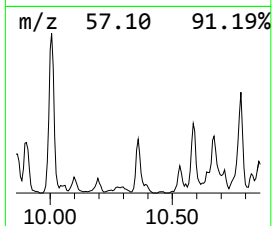
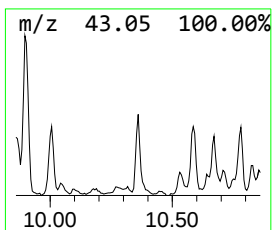
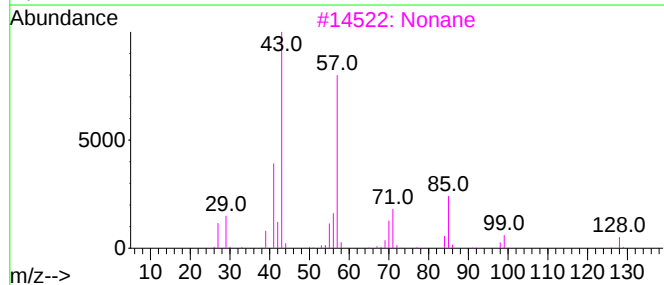
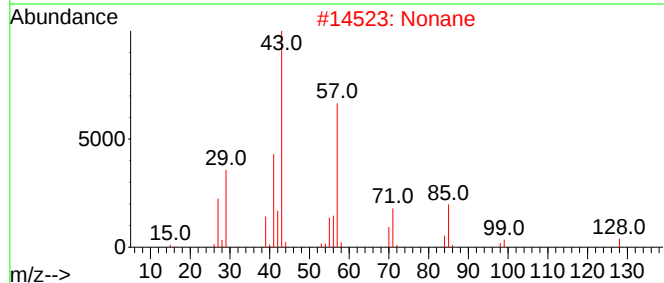
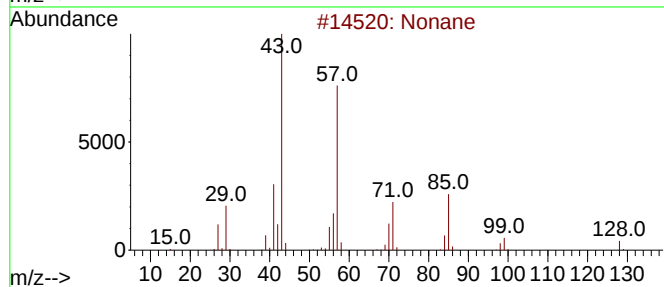
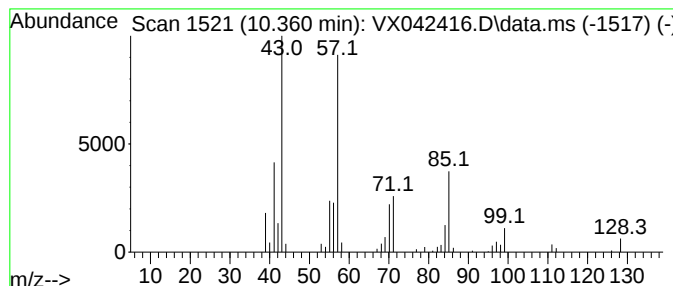
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	3.04 ug/L	39628	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	87
2			Nonane	128	C9H20	000111-84-2	87
3			Nonane	128	C9H20	000111-84-2	72
4			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	49
5			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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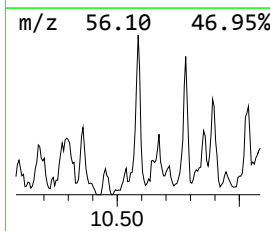
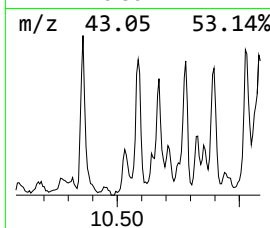
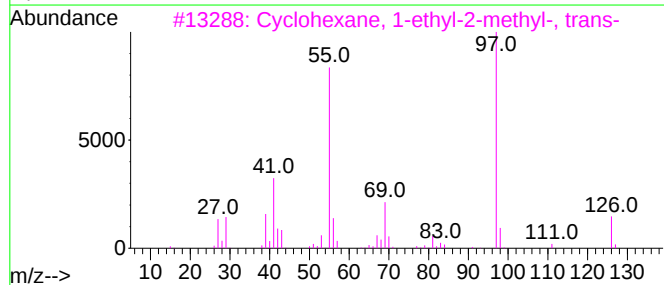
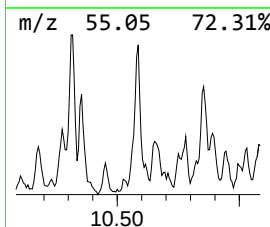
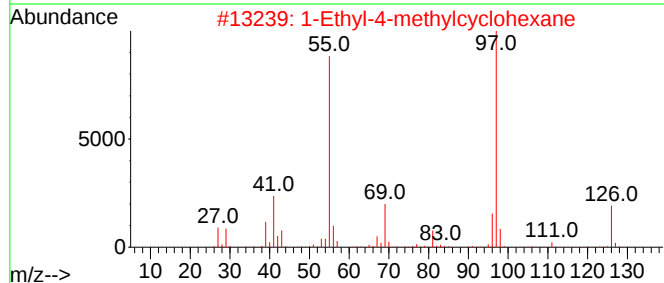
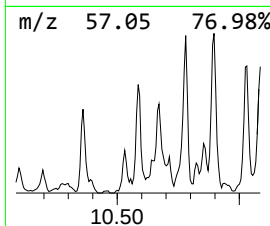
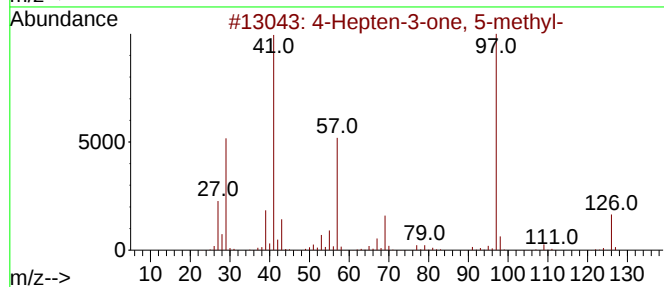
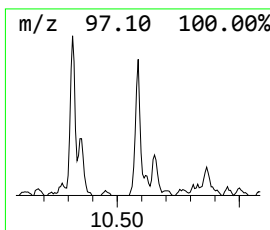
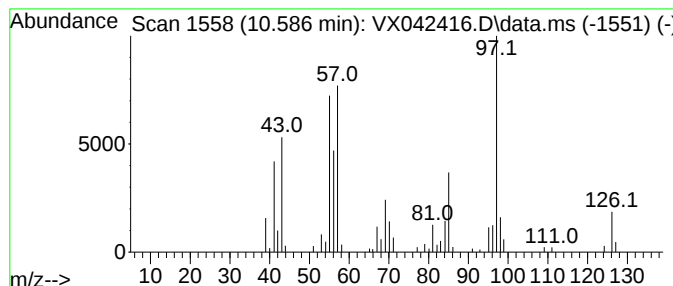
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	4.49 ug/L	58491	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Hepten-3-one, 5-methyl-	126	C8H14O	001447-26-3	43
2			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	43
3			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	43
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	43
5			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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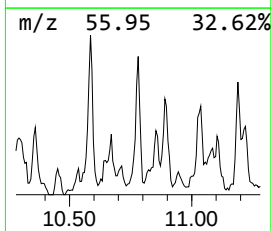
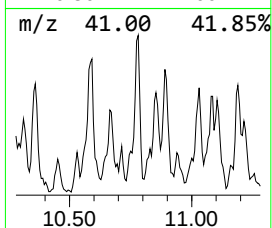
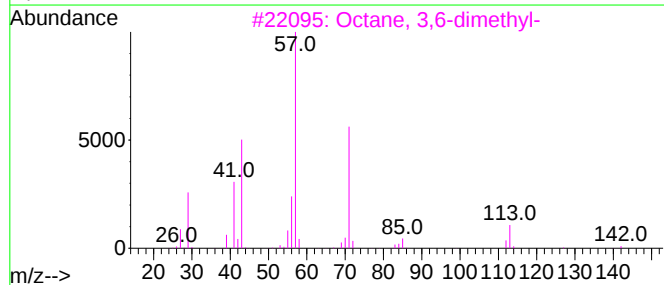
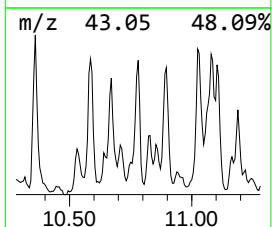
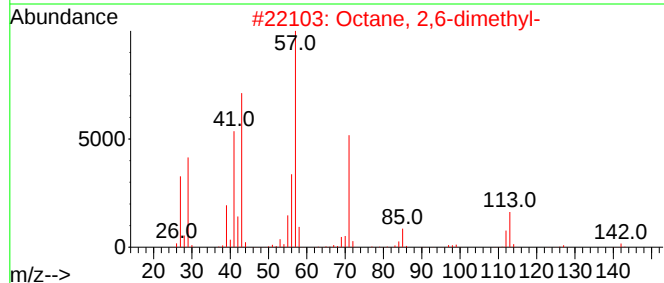
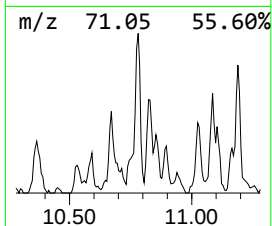
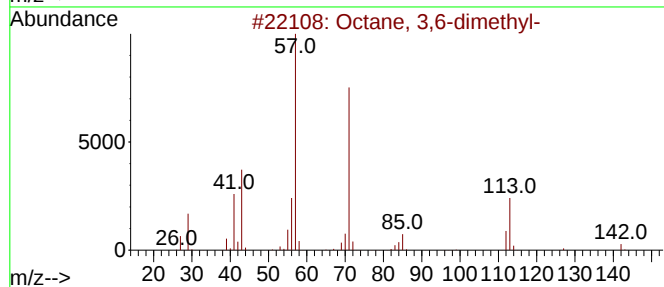
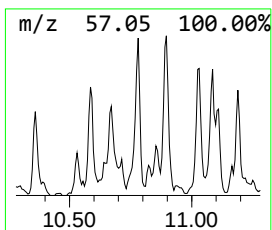
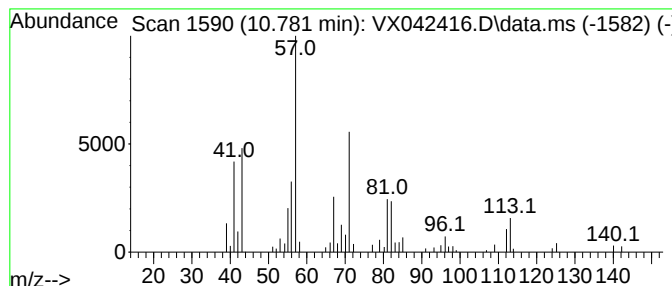
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	4.43 ug/L	57746	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-			142	C10H22	015869-94-0	64
2	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	64
3	Octane, 3,6-dimethyl-			142	C10H22	015869-94-0	53
4	Nonane, 3-methyl-			142	C10H22	005911-04-6	52
5	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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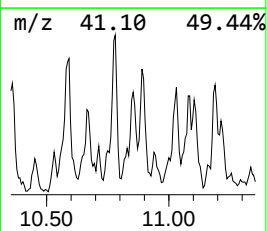
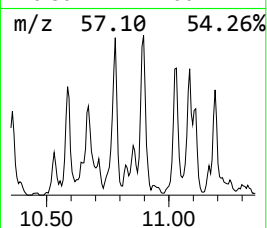
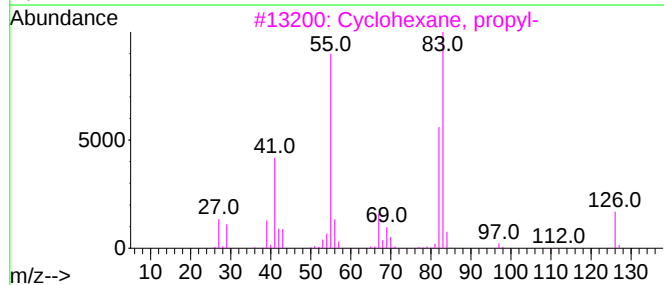
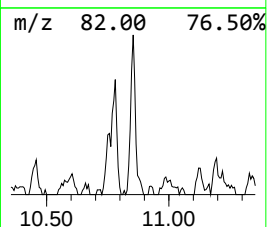
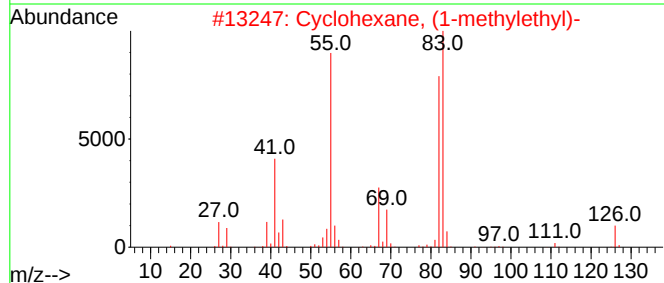
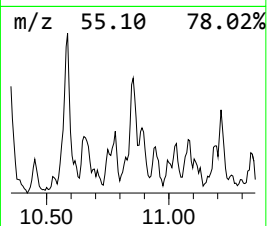
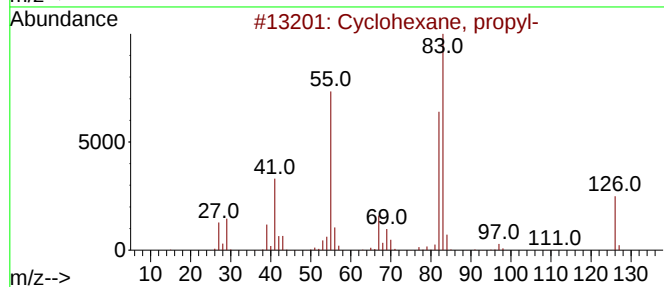
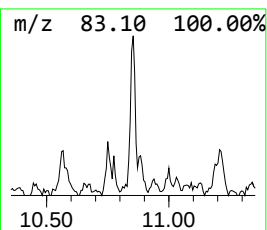
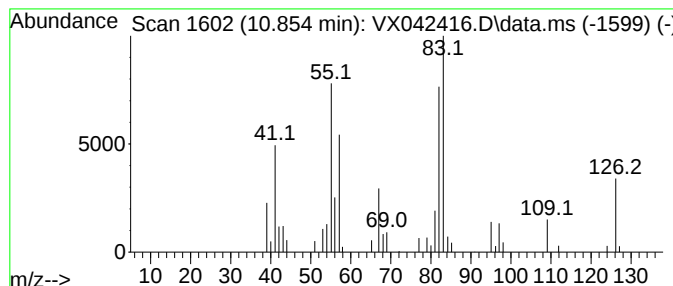
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Quant Title : VOC Analysis

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

Peak Number 10 (DEL) Alkane: Cyclic10.854 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	2.67 ug/L	34755	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	72
2			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72
3			Cyclohexane, propyl-	126	C9H18	001678-92-8	64
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	64
5			n-Heptadecylcyclohexane	322	C23H46	019781-73-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

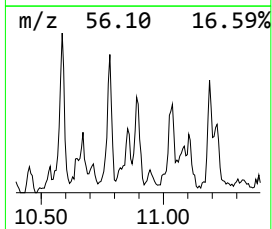
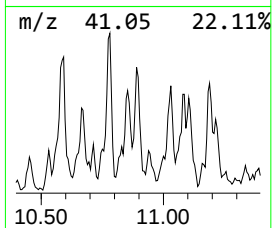
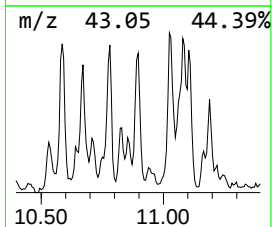
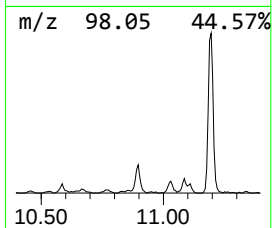
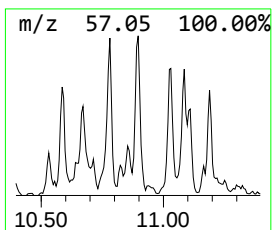
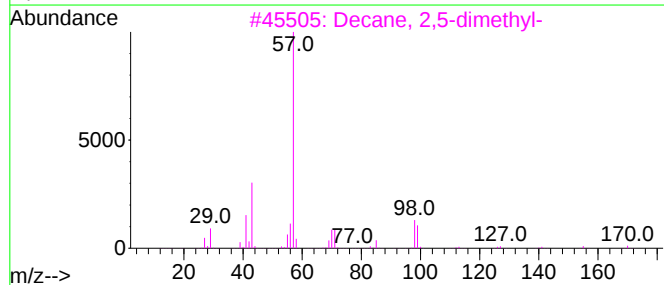
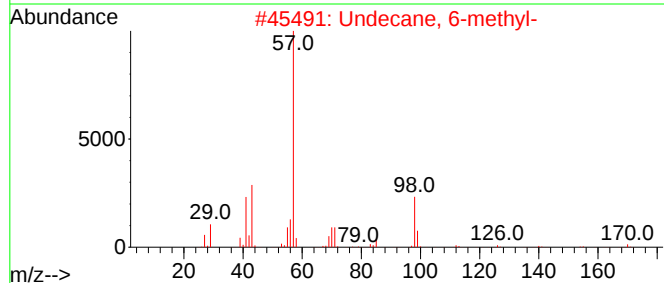
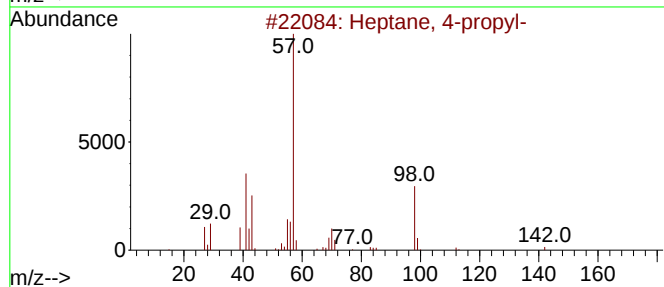
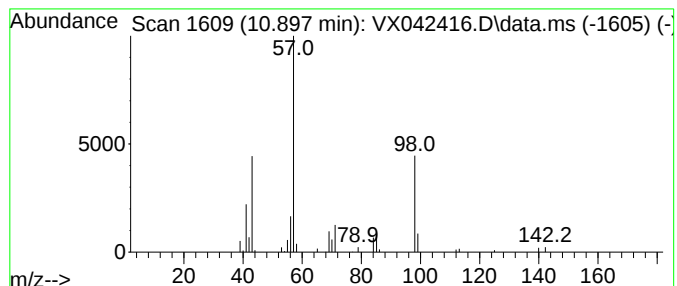
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Quant Title : VOC Analysis

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

Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.897	2.99 ug/L	38946	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 4-propyl-	142	C10H22	003178-29-8	78
2			Undecane, 6-methyl-	170	C12H26	017302-33-9	53
3			Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	53
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

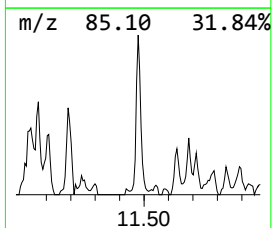
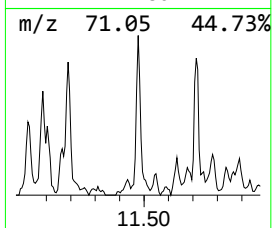
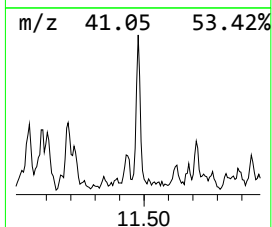
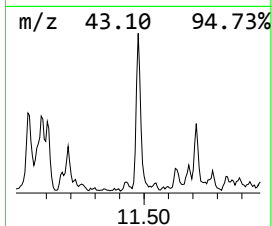
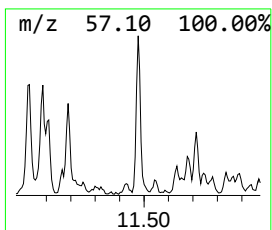
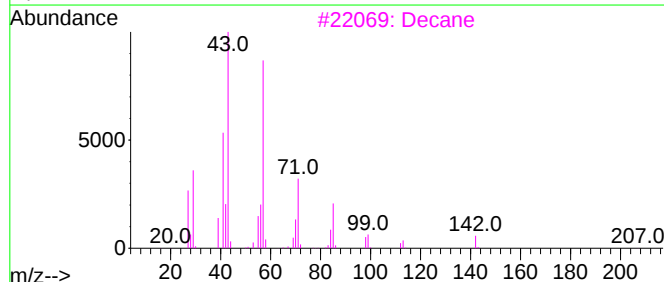
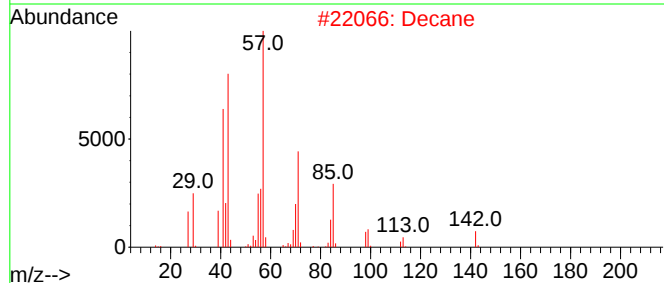
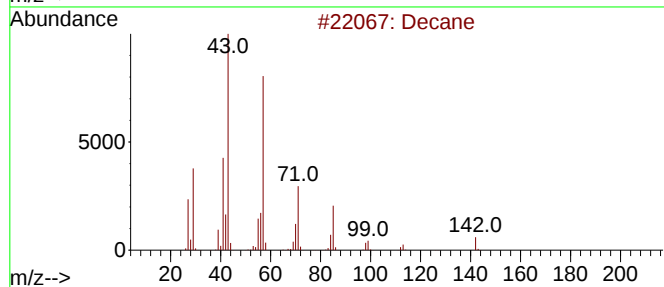
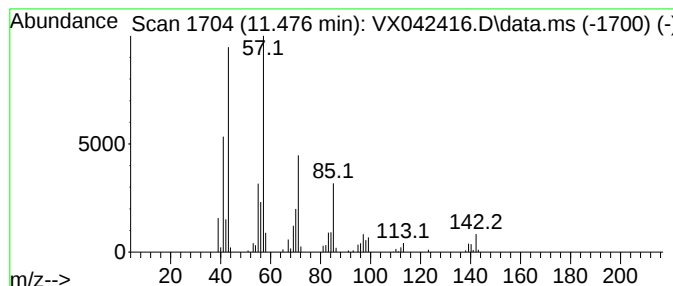
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Quant Title : VOC Analysis

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

Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.476	3.83 ug/L	50577	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	93
2			Decane	142	C10H22	000124-18-5	93
3			Decane	142	C10H22	000124-18-5	87
4			Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	86
5			Decane	142	C10H22	000124-18-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

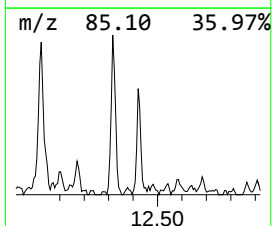
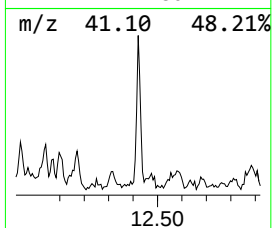
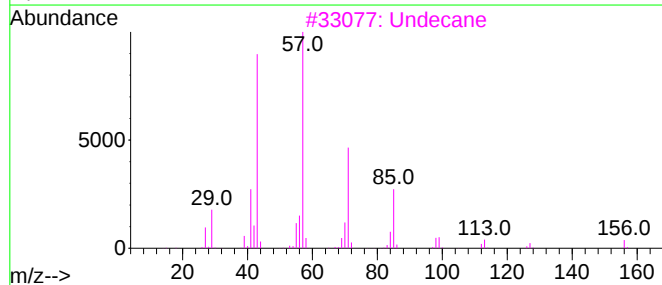
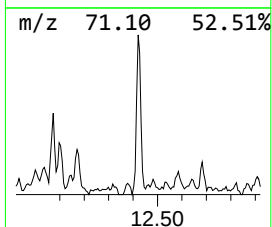
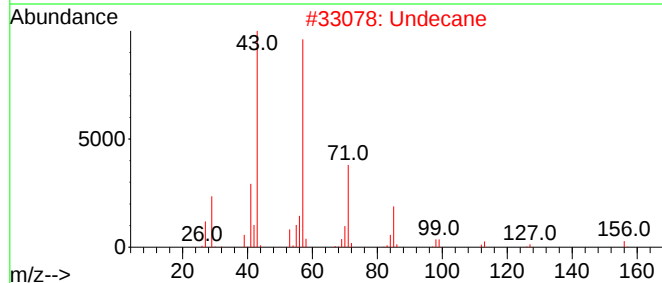
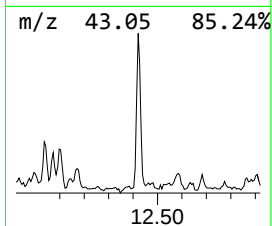
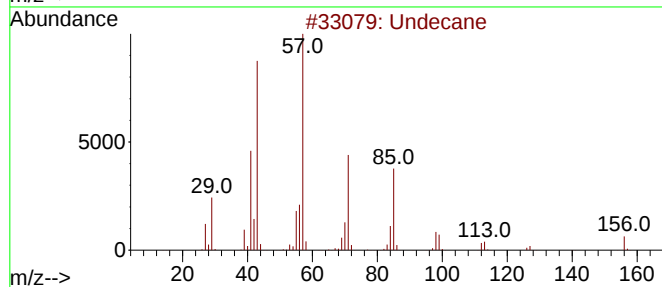
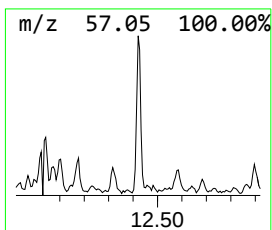
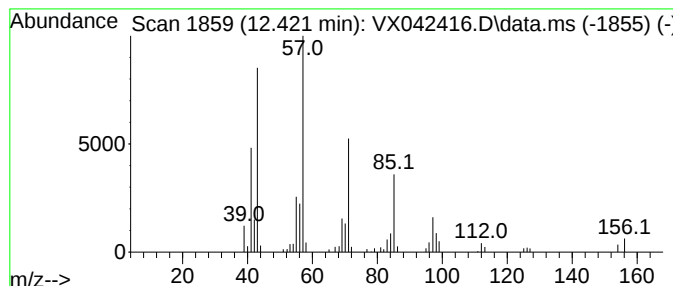
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Quant Title : VOC Analysis

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

Peak Number 13 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	2.89 ug/L	38099	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	72
2	Undecane			156	C11H24	001120-21-4	70
3	Undecane			156	C11H24	001120-21-4	68
4	Hydroxylamine, O-decyl-			173	C10H23NO	029812-79-1	59
5	Tetradecane			198	C14H30	000629-59-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

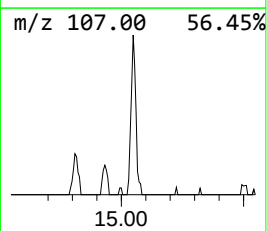
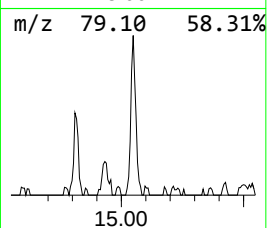
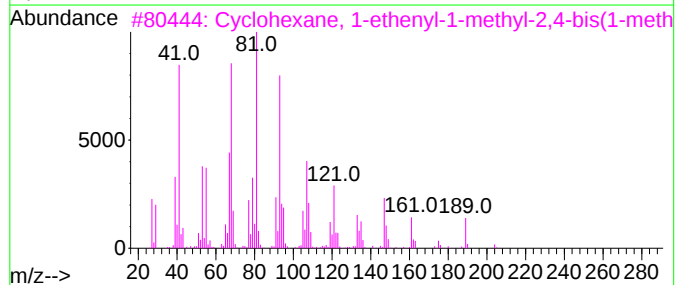
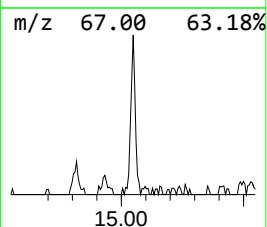
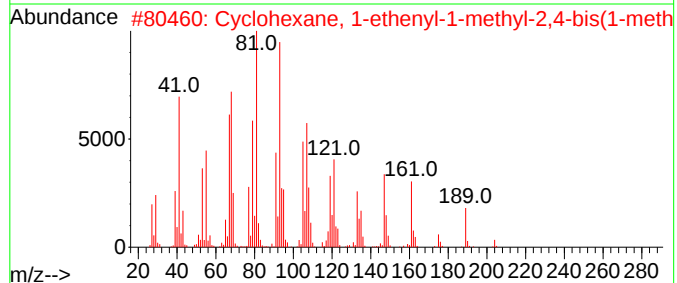
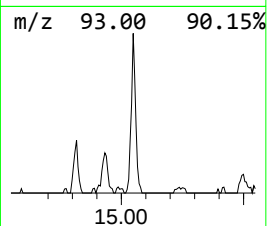
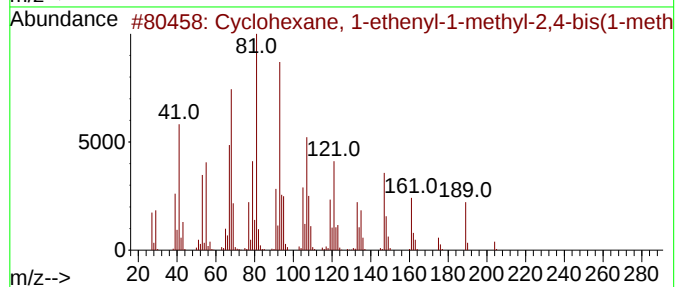
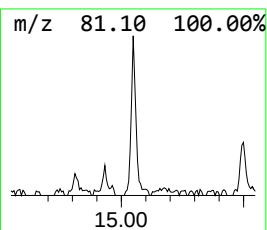
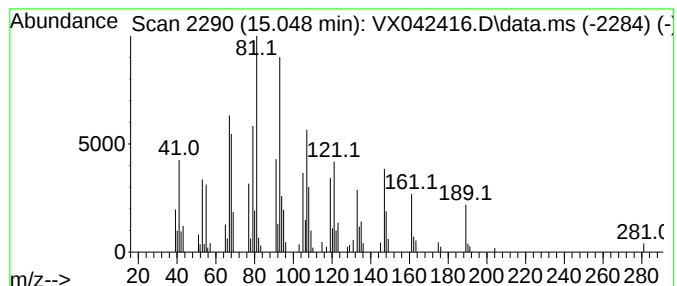
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Quant Title : VOC Analysis

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

Peak Number 14 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.048	3.49 ug/L	46080	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	91
2			Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	90
3			Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	033880-83-0	81
4			Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	110823-68-2	64
5			1,5,9-Cyclododecatriene, 1,5,9-t...	204	C15H24	021064-19-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042416.D
Acq On : 19 Jul 2024 20:48
Operator : JC/MD
Sample : P3238-19ME
Misc : 4.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CH4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	3.5	ug/L	37743	1	6.757	542948	50.0
(DEL) Alkane: C...	9.500	3.8	ug/L	49233	2	10.055	651848	50.0
(DEL) Alkane: C...	9.616	6.0	ug/L	78424	2	10.055	651848	50.0
(DEL) Alkane: C...	9.830	3.6	ug/L	47638	2	10.055	651848	50.0
(DEL) Alkane: S...	9.897	3.3	ug/L	43530	2	10.055	651848	50.0
(DEL) Alkane: S...	10.360	3.0	ug/L	39628	2	10.055	651848	50.0
unknown-01	10.586	4.5	ug/L	58491	2	10.055	651848	50.0
(DEL) Alkane: S...	10.781	4.4	ug/L	57746	2	10.055	651848	50.0
(DEL) Alkane: C...	10.854	2.7	ug/L	34755	2	10.055	651848	50.0
(DEL) Alkane: S...	10.897	3.0	ug/L	38946	2	10.055	651848	50.0
(DEL) Alkane: S...	11.476	3.8	ug/L	50577	3	12.024	659792	50.0
(DEL) Alkane: S...	12.421	2.9	ug/L	38099	3	12.024	659792	50.0
Cyclohexane, 1-...	15.048	3.5	ug/L	46080	3	12.024	659792	50.0