

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
 Data File : VX036946.D
 Acq On : 11 Aug 2023 17:15
 Operator : JC/MD
 Sample : 03903-10 10X
 Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-10

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036946.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.581	69	81	82	rBV6	3611	11301	1.63%	0.184%
2	4.593	563	575	586	rBV2	7441	24712	3.57%	0.401%
3	5.385	692	705	717	rBV	76845	225032	32.53%	3.656%
4	5.550	718	732	751	rVB	125603	370139	53.50%	6.013%
5	5.824	769	777	787	rBV5	4222	12889	1.86%	0.209%
6	5.958	787	799	819	rVV	79354	215657	31.17%	3.504%
7	6.160	823	832	839	rVV8	2599	7905	1.14%	0.128%
8	6.251	839	847	856	rVB4	3595	11285	1.63%	0.183%
9	6.763	922	931	942	rBV	203888	486047	70.26%	7.896%
10	7.373	1022	1031	1043	rVB4	12035	32255	4.66%	0.524%
11	7.495	1043	1051	1057	rBV3	4420	9546	1.38%	0.155%
12	7.562	1057	1062	1073	rVB4	5294	11493	1.66%	0.187%
13	7.775	1090	1097	1103	rVB3	9951	19696	2.85%	0.320%
14	7.958	1120	1127	1139	rVB6	7970	21605	3.12%	0.351%
15	8.190	1159	1165	1169	rBV4	6007	11790	1.70%	0.192%
16	8.275	1174	1179	1182	rVV2	9983	18056	2.61%	0.293%
17	8.312	1182	1185	1192	rVB4	12881	23117	3.34%	0.376%
18	8.434	1201	1205	1214	rVV2	11469	25954	3.75%	0.422%
19	8.519	1214	1219	1225	rVB3	5215	10636	1.54%	0.173%
20	8.598	1225	1232	1235	rBV3	29205	52676	7.61%	0.856%
21	8.647	1235	1240	1251	rVV	436289	691826	100.00%	11.240%
22	8.775	1255	1261	1265	rVV2	15761	27044	3.91%	0.439%
23	8.818	1265	1268	1270	rVV2	6503	9177	1.33%	0.149%
24	8.848	1270	1273	1278	rVB4	5974	9356	1.35%	0.152%
25	8.976	1288	1294	1300	rVB2	31218	50680	7.33%	0.823%
26	9.104	1306	1315	1320	rBV	22525	37574	5.43%	0.610%
27	9.159	1320	1324	1328	rBV2	8307	12928	1.87%	0.210%
28	9.293	1339	1346	1350	rVB2	7971	12711	1.84%	0.207%
29	9.385	1356	1361	1372	rBV2	20139	34159	4.94%	0.555%
30	9.500	1375	1380	1386	rBV3	28005	55195	7.98%	0.897%
31	9.561	1386	1390	1395	rVB	20287	27726	4.01%	0.450%
32	9.616	1395	1399	1403	rBV	30258	48021	6.94%	0.780%
33	9.659	1403	1406	1409	rVV2	7654	11118	1.61%	0.181%
34	9.695	1409	1412	1417	rVB4	5698	8540	1.23%	0.139%
35	9.763	1417	1423	1427	rBV4	8758	14142	2.04%	0.230%
36	9.830	1427	1434	1438	rBV3	26016	53998	7.81%	0.877%

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37	9.903	1442	1446	1455	rVB2	22722	36445	5.27%	0.592%
38	10.006	1456	1463	1466	rBV	21529	33678	4.87%	0.547%
39	10.055	1466	1471	1477	rVB	454057	593382	85.77%	9.640%
40	10.122	1480	1482	1487	rVB3	7984	10545	1.52%	0.171%
41	10.189	1487	1493	1498	rBV4	13331	26235	3.79%	0.426%
42	10.275	1502	1507	1509	rBV2	17771	27965	4.04%	0.454%
43	10.317	1509	1514	1517	rVB2	29646	58101	8.40%	0.944%
44	10.354	1517	1520	1531	rVB4	17950	37555	5.43%	0.610%
45	10.458	1531	1537	1545	rBV2	12858	21592	3.12%	0.351%
46	10.586	1551	1558	1566	rBV4	40243	77672	11.23%	1.262%
47	10.671	1566	1572	1577	rBV4	19803	34883	5.04%	0.567%
48	10.714	1577	1579	1582	rVB2	7596	7148	1.03%	0.116%
49	10.781	1586	1590	1594	rVB	57760	72926	10.54%	1.185%
50	10.854	1594	1602	1606	rBV3	48419	77796	11.25%	1.264%
51	10.890	1606	1608	1614	rVB2	20488	28135	4.07%	0.457%
52	10.951	1614	1618	1622	rVB5	6121	10964	1.58%	0.178%
53	11.006	1622	1627	1628	rBV4	11252	17243	2.49%	0.280%
54	11.031	1628	1631	1634	rVB2	16342	19328	2.79%	0.314%
55	11.079	1634	1639	1645	rBV	406988	497935	71.97%	8.090%
56	11.189	1654	1657	1659	rVV4	11662	13565	1.96%	0.220%
57	11.220	1659	1662	1666	rVB3	19430	23110	3.34%	0.375%
58	11.305	1672	1676	1678	rBV	7495	9639	1.39%	0.157%
59	11.335	1678	1681	1684	rVV4	8430	12591	1.82%	0.205%
60	11.384	1684	1689	1694	rVV5	23752	41135	5.95%	0.668%
61	11.433	1694	1697	1702	rBV2	16543	31059	4.49%	0.505%
62	11.524	1710	1712	1718	rVB6	5004	7216	1.04%	0.117%
63	11.628	1722	1729	1734	rBV4	20030	43586	6.30%	0.708%
64	11.683	1734	1738	1740	rVV3	18286	23976	3.47%	0.390%
65	11.713	1740	1743	1746	rVV	56911	67202	9.71%	1.092%
66	11.750	1746	1749	1759	rVB2	52508	105649	15.27%	1.716%
67	11.835	1759	1763	1766	rBV3	17640	27588	3.99%	0.448%
68	11.890	1769	1772	1776	rVB2	24162	30770	4.45%	0.500%
69	11.939	1776	1780	1783	rBV2	11008	16658	2.41%	0.271%
70	11.976	1783	1786	1788	rVV3	9243	9758	1.41%	0.159%
71	12.024	1788	1794	1800	rVV	451148	606151	87.62%	9.848%
72	12.073	1800	1802	1811	rVB3	9935	20691	2.99%	0.336%
73	12.250	1826	1831	1836	rBV2	22708	42346	6.12%	0.688%
74	12.311	1836	1841	1848	rVV3	29127	61909	8.95%	1.006%
75	12.469	1864	1867	1872	rVB6	10897	21344	3.09%	0.347%
76	12.536	1875	1878	1879	rBV2	9006	10143	1.47%	0.165%

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77	12.579	1882	1885	1888	rVV3	14083	20662	2.99%	0.336%
78	12.616	1888	1891	1894	rVB	24332	26654	3.85%	0.433%
79	12.683	1899	1902	1909	rVV3	11342	20116	2.91%	0.327%
80	12.817	1919	1924	1930	rVB3	23582	42810	6.19%	0.696%
81	12.896	1930	1937	1938	rBV4	16262	26511	3.83%	0.431%
82	12.921	1938	1941	1947	rVV2	35730	51177	7.40%	0.831%
83	12.981	1948	1951	1955	rVV5	11102	15990	2.31%	0.260%
84	13.030	1955	1959	1964	rVB4	13860	29023	4.20%	0.472%
85	13.091	1964	1969	1974	rBV7	6890	17332	2.51%	0.282%
86	13.292	1998	2002	2008	rVB2	39210	56976	8.24%	0.926%
87	13.384	2012	2017	2020	rBV2	14516	22796	3.30%	0.370%
88	13.506	2033	2037	2040	rBV5	6954	10545	1.52%	0.171%
89	13.542	2040	2043	2046	rVV	11164	13483	1.95%	0.219%
90	13.585	2046	2050	2054	rVV3	22981	31464	4.55%	0.511%
91	13.664	2060	2063	2068	rVB2	17669	26885	3.89%	0.437%
92	13.725	2070	2073	2078	rVB7	6048	7807	1.13%	0.127%
93	13.774	2078	2081	2083	rBV	7113	7682	1.11%	0.125%
94	13.841	2088	2092	2098	rVB5	14776	23545	3.40%	0.383%
95	13.920	2099	2105	2110	rVB9	9207	16199	2.34%	0.263%
96	13.969	2110	2113	2117	rBV3	8378	11362	1.64%	0.185%
97	14.073	2125	2130	2134	rBV	11740	17051	2.46%	0.277%
98	14.213	2149	2153	2160	rVB3	16019	20815	3.01%	0.338%
99	14.371	2176	2179	2183	rVB	8429	9684	1.40%	0.157%
100	14.481	2193	2197	2201	rBV4	4558	7066	1.02%	0.115%

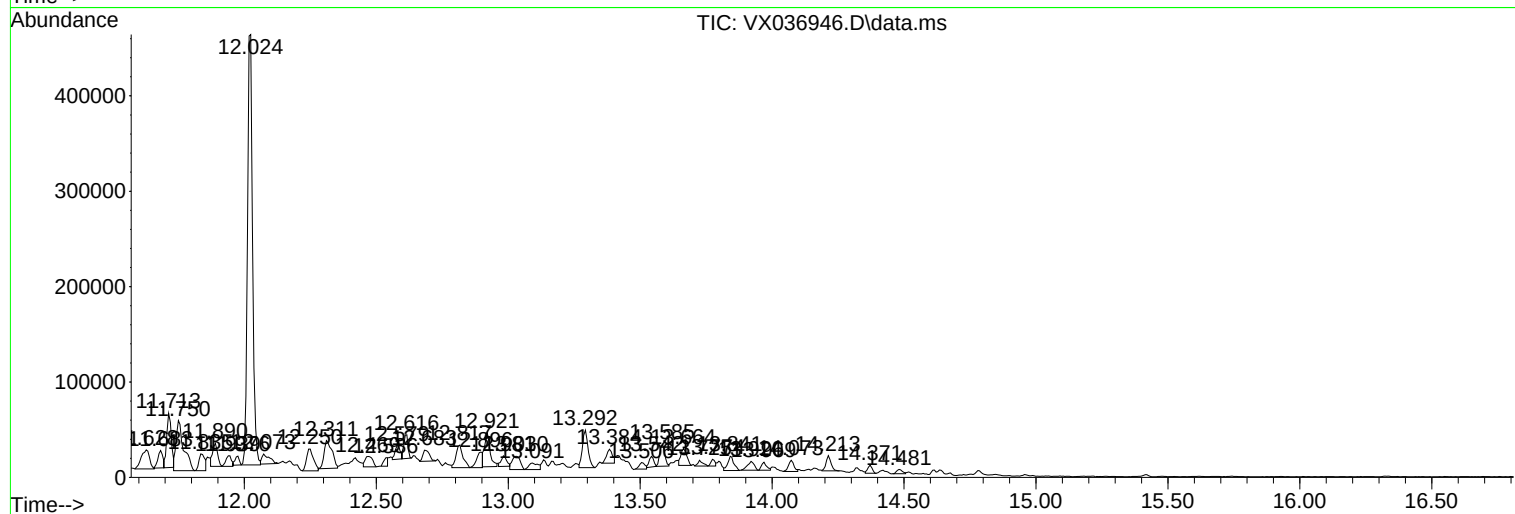
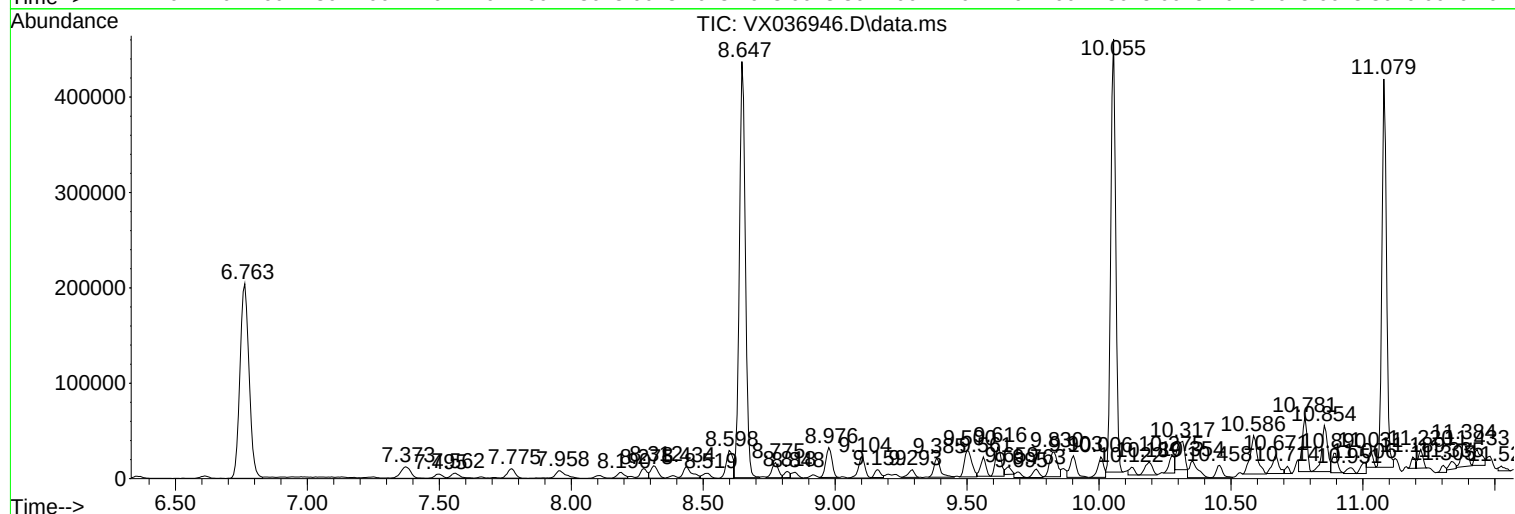
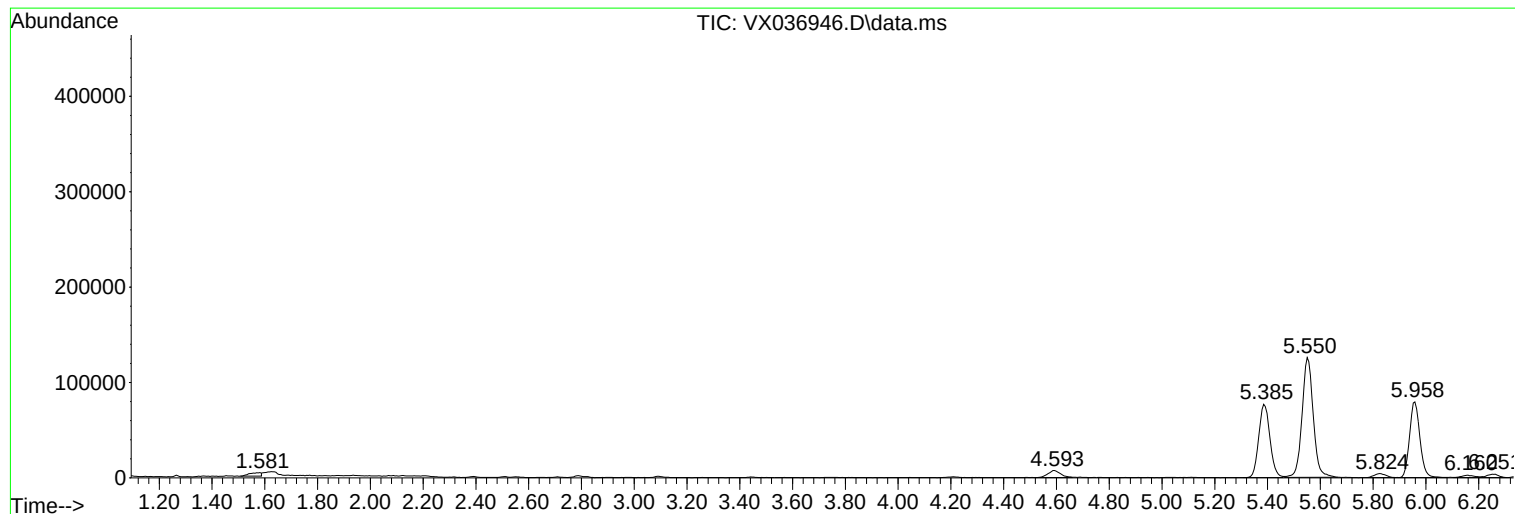
Sum of corrected areas: 6155235

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MSVOA_X
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MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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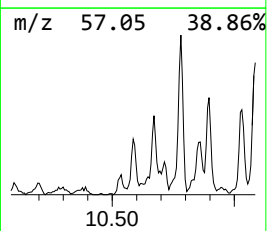
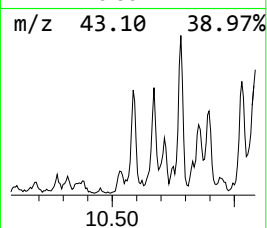
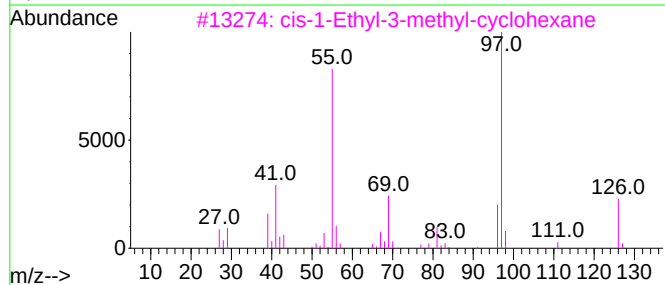
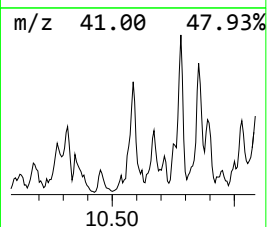
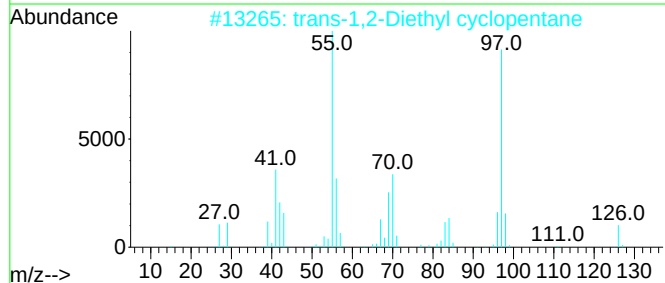
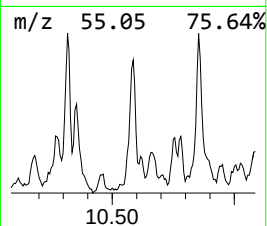
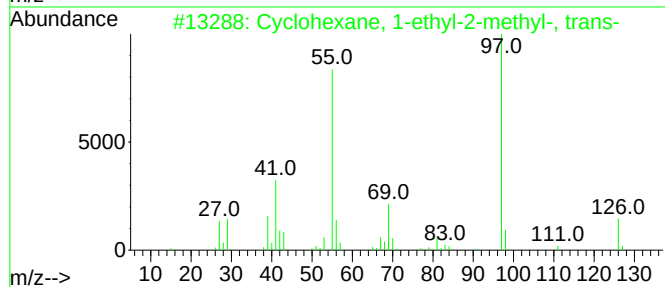
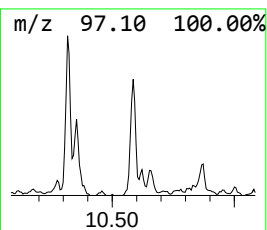
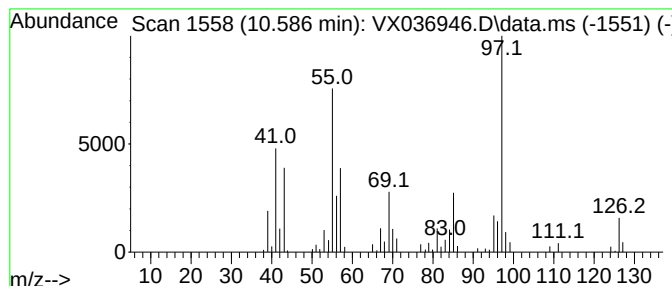
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	6.54 ug/l	77672	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	70
2			trans-1,2-Diethyl cyclopentane	126	C9H18	000932-40-1	64
3			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	62
4			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	58
5			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	58



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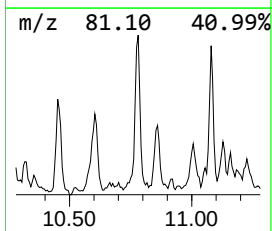
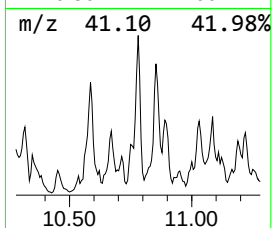
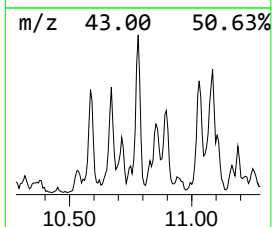
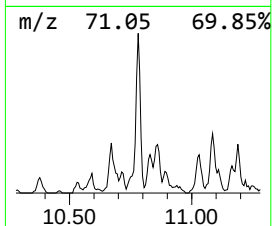
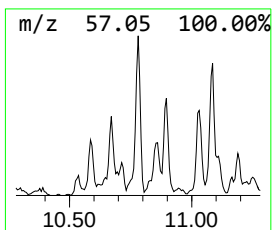
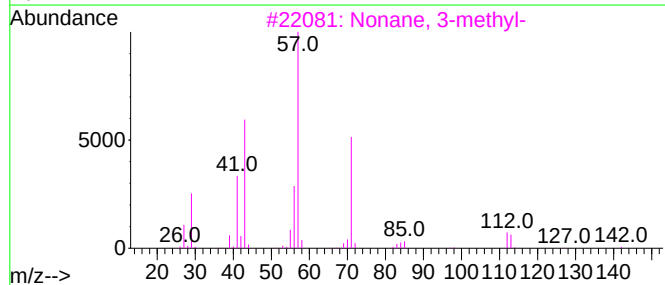
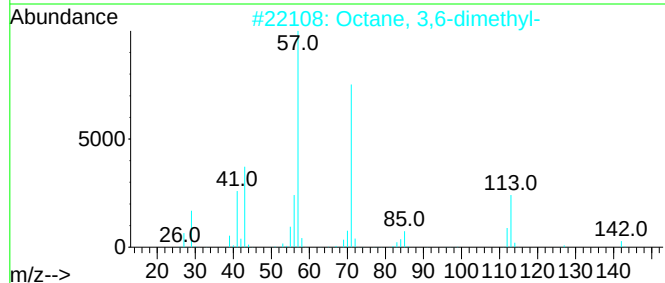
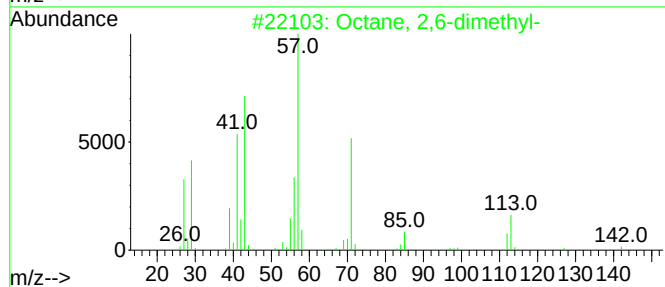
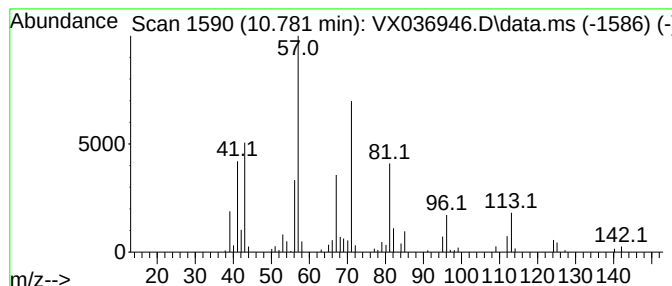
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Quant Title : SW846 8260

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

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	6.14 ug/l	72926	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	70
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	62
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	43
5			2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	43



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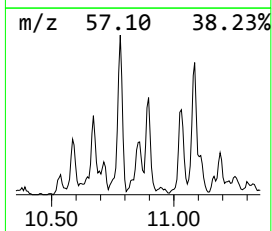
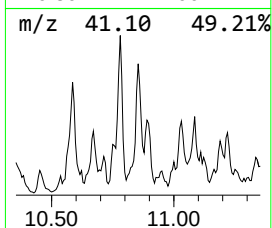
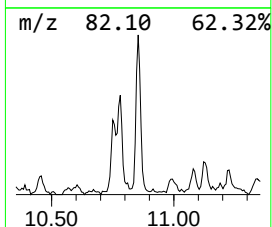
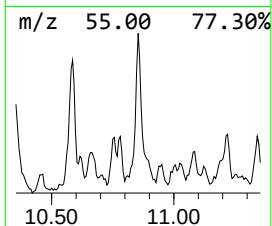
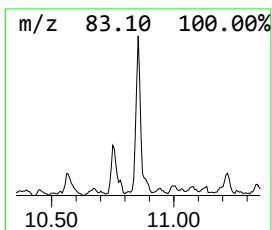
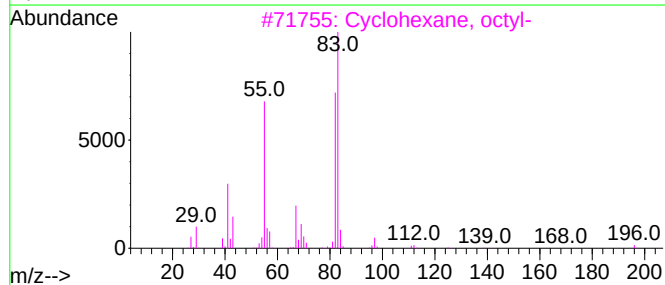
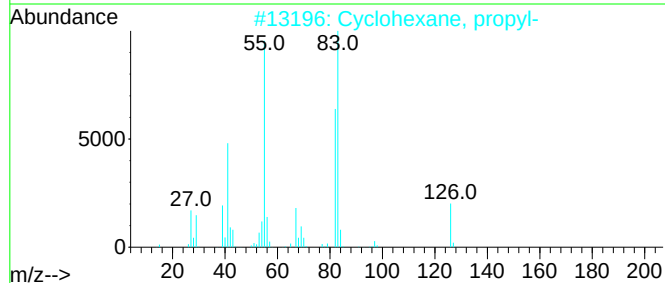
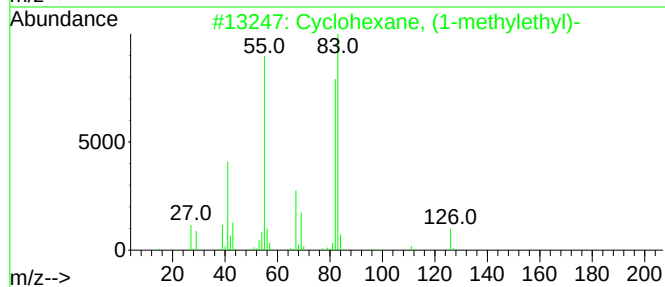
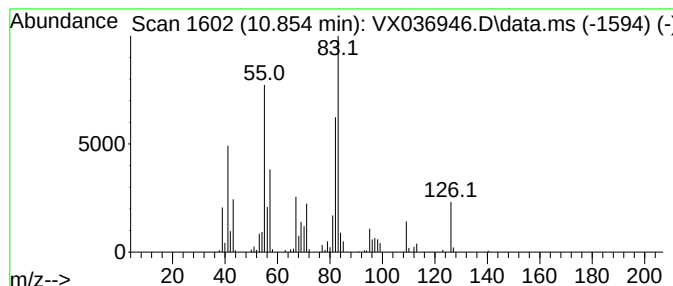
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, (1-methylethyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	6.56 ug/l	77796	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	76
2			Cyclohexane, propyl-	126	C9H18	001678-92-8	76
3			Cyclohexane, octyl-	196	C14H28	001795-15-9	53
4			Cyclohexane, butyl-	140	C10H20	001678-93-9	53
5			Cyclohexane, 1,1'-(1,4-butanedi...	222	C16H30	006165-44-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036946.D
Acq On : 11 Aug 2023 17:15
Operator : JC/MD
Sample : 03903-10 10X
Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

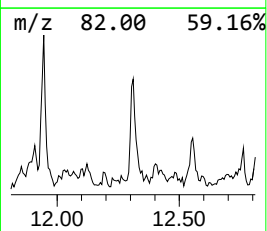
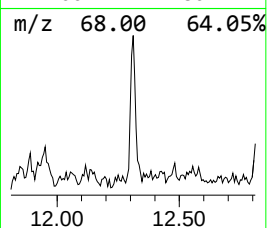
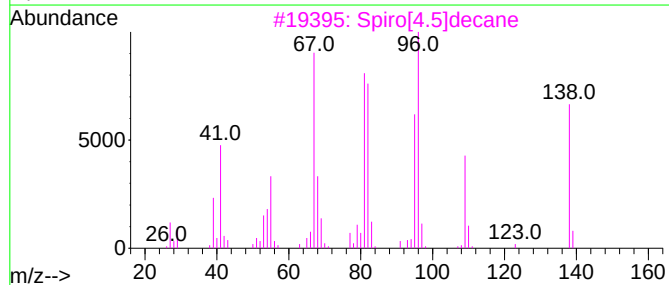
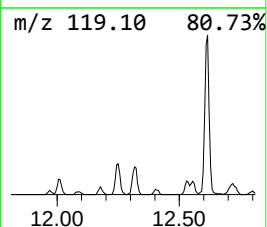
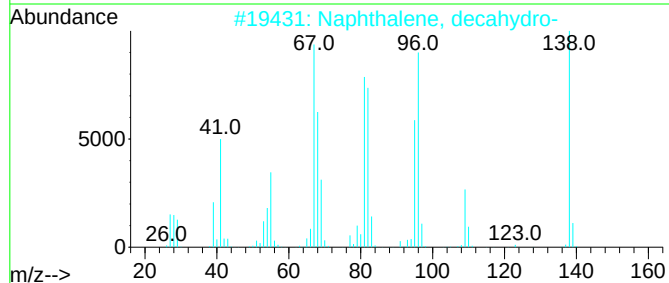
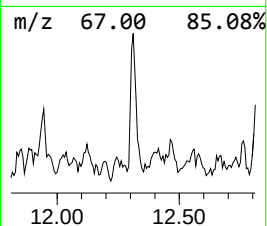
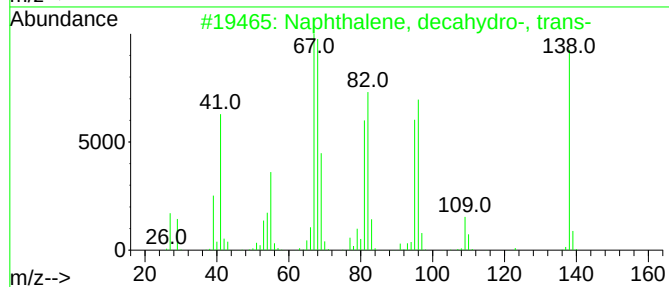
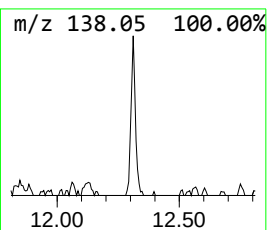
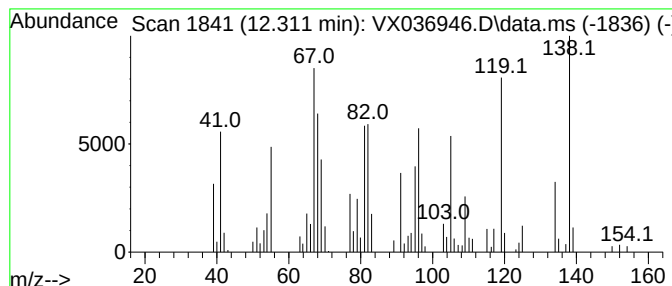
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, decahydro-, tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.311	5.11 ug/l	61909	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3			Spiro[4.5]decane	138	C10H18	000176-63-6	86
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	86
5			2,2-Dimethyl-3-vinylcyclopentanone	138	C9H14O	1000427-24-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036946.D
Acq On : 11 Aug 2023 17:15
Operator : JC/MD
Sample : 03903-10 10X
Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1-...	10.586	6.5	ug/l	77672	3	10.055	593382	50.0
Octane, 2,6-dim...	10.781	6.1	ug/l	72926	3	10.055	593382	50.0
Cyclohexane, (1...	10.854	6.6	ug/l	77796	3	10.055	593382	50.0
Naphthalene, de...	12.311	5.1	ug/l	61909	4	12.024	606151	50.0