

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD031622\
 Data File : VD072222.D
 Acq On : 16 Mar 2022 17:02
 Operator : VA/SY
 Sample : N1914-04
 Misc : 5.07G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 TP-2

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_D\Method\82D031122S.M
 Title : SW846 8260

Signal : TIC: VD072222.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.961	503	517	531	rBV5	52961	185221	6.13%	0.858%
2	5.991	682	692	702	rVB5	20030	61408	2.03%	0.284%
3	7.908	1006	1018	1023	rBV	354238	834197	27.61%	3.863%
4	7.973	1023	1029	1038	rVV	710247	1641748	54.34%	7.603%
5	8.061	1038	1044	1055	rVB2	69754	178441	5.91%	0.826%
6	8.326	1081	1089	1099	rVB	304273	667904	22.11%	3.093%
7	8.444	1103	1109	1117	rBV3	20587	42357	1.40%	0.196%
8	8.861	1170	1180	1191	rBV	1014535	2062388	68.27%	9.551%
9	9.320	1247	1258	1268	rBV5	105530	334013	11.06%	1.547%
10	9.402	1268	1272	1279	rVB3	50365	93376	3.09%	0.432%
11	9.620	1297	1309	1317	rBV2	132123	301468	9.98%	1.396%
12	9.773	1327	1335	1347	rVB5	37326	78917	2.61%	0.365%
13	9.908	1349	1358	1363	rVV4	27576	60907	2.02%	0.282%
14	9.955	1363	1366	1373	rVB4	24454	43624	1.44%	0.202%
15	10.091	1381	1389	1394	rBV3	61985	125359	4.15%	0.581%
16	10.138	1394	1397	1405	rVB4	15871	30940	1.02%	0.143%
17	10.226	1405	1412	1422	rBV8	25742	91364	3.02%	0.423%
18	10.332	1422	1430	1446	rBV	1650517	3021123	100.00%	13.991%
19	10.508	1453	1460	1470	rVB4	58756	154835	5.13%	0.717%
20	10.632	1470	1481	1484	rBV4	69428	145591	4.82%	0.674%
21	10.673	1484	1488	1496	rVV2	139775	256297	8.48%	1.187%
22	10.773	1498	1505	1509	rVV6	44157	104610	3.46%	0.484%
23	10.814	1509	1512	1515	rVV5	30779	51626	1.71%	0.239%
24	10.861	1515	1520	1524	rVV2	49561	86079	2.85%	0.399%
25	10.920	1524	1530	1533	rVV5	17273	42558	1.41%	0.197%
26	11.043	1541	1551	1560	rVV2	90157	232678	7.70%	1.078%
27	11.120	1560	1564	1567	rVV3	38832	73689	2.44%	0.341%
28	11.155	1567	1570	1576	rVV3	54178	94076	3.11%	0.436%
29	11.238	1576	1584	1589	rVV3	134803	291708	9.66%	1.351%
30	11.296	1589	1594	1597	rVV3	63183	122189	4.04%	0.566%
31	11.338	1597	1601	1606	rVV4	85454	169617	5.61%	0.786%
32	11.390	1606	1610	1614	rVV3	34817	64334	2.13%	0.298%
33	11.443	1614	1619	1628	rVB	104745	187690	6.21%	0.869%
34	11.637	1644	1652	1663	rVV	1623274	2854498	94.48%	13.219%
35	11.773	1670	1675	1679	rBV4	42544	61270	2.03%	0.284%
36	11.826	1679	1684	1689	rBV5	47998	85849	2.84%	0.398%

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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 >

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37	11.885	1689	1694	1696	rBV2	44011	75902	2.51%	0.352%
38	11.985	1706	1711	1716	rBV7	35611	76414	2.53%	0.354%
39	12.149	1731	1739	1745	rBV3	124601	301470	9.98%	1.396%
40	12.232	1749	1753	1761	rVB8	45649	110230	3.65%	0.510%
41	12.314	1761	1767	1768	rBV3	44814	79259	2.62%	0.367%
42	12.349	1768	1773	1775	rBV4	84389	146199	4.84%	0.677%
43	12.620	1812	1819	1827	rVB	1315733	2269532	75.12%	10.510%
44	12.708	1827	1834	1839	rBV9	31386	81817	2.71%	0.379%
45	12.784	1842	1847	1854	rVB2	132260	255035	8.44%	1.181%
46	12.873	1854	1862	1866	rBV7	44079	106868	3.54%	0.495%
47	12.943	1868	1874	1881	rBV10	49429	139294	4.61%	0.645%
48	13.084	1895	1898	1902	rVB3	30483	40341	1.34%	0.187%
49	13.561	1972	1979	1988	rBV	1739055	2833864	93.80%	13.124%
50	13.702	1999	2003	2008	rVB5	21569	33997	1.13%	0.157%
51	13.884	2028	2034	2040	rVB8	32919	56931	1.88%	0.264%
52	15.384	2280	2289	2297	rVB2	22168	52193	1.73%	0.242%

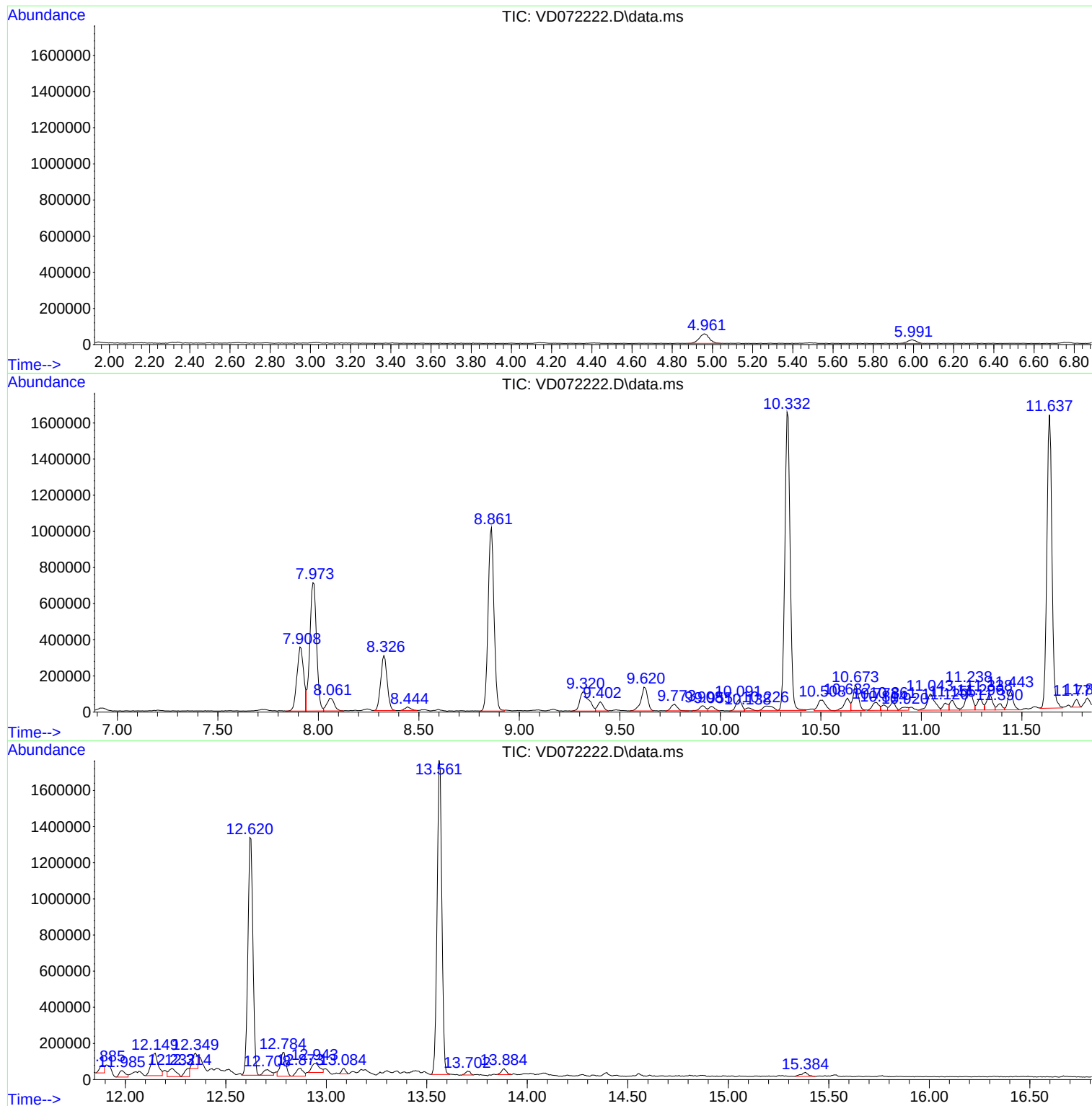
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MSVOA_D
ClientSampleId :
TP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031122S.M
Quant Title : SW846 8260

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



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TP-2

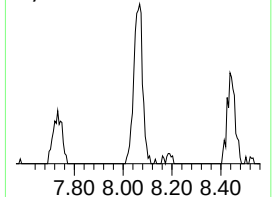
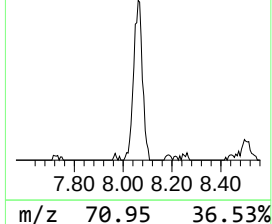
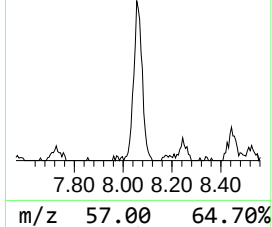
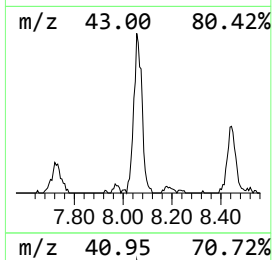
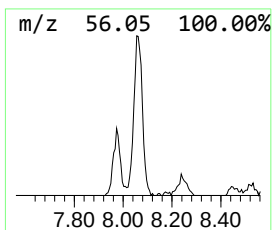
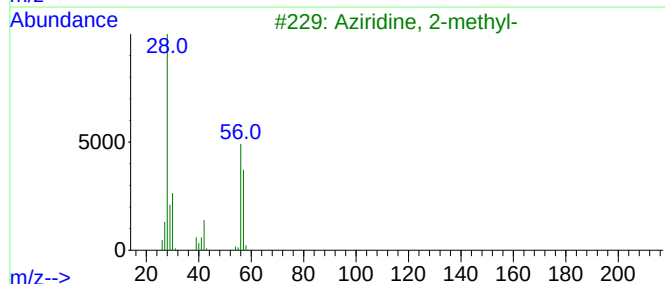
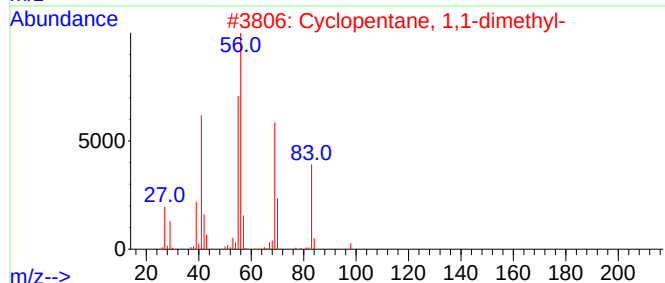
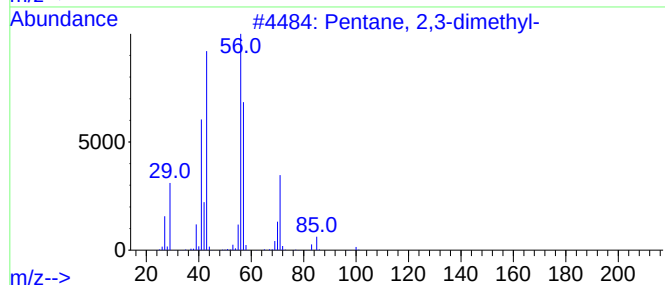
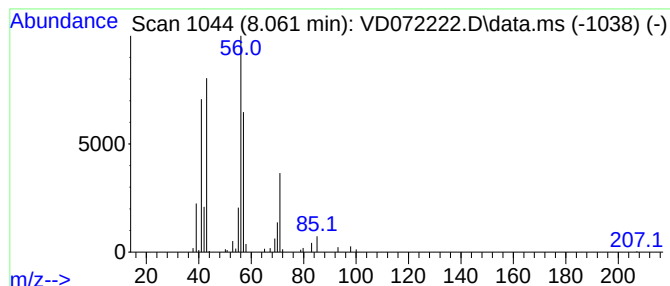
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031122S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.061	5.43 ug/l	178441	Pentafluorobenzene	7.979

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	40
4			cis-4,6-Dimethylcyclohexane-1,3-...	140	C8H12O2	069841-15-2	40
5			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40



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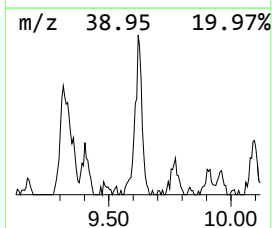
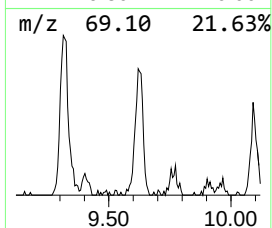
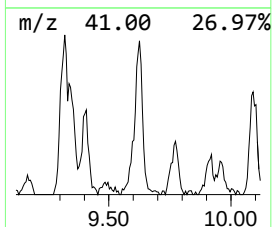
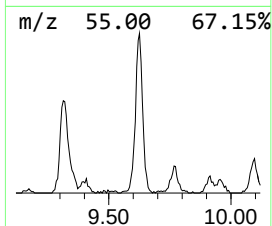
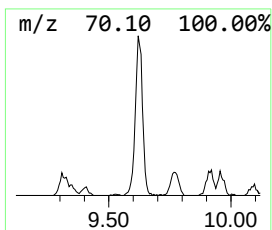
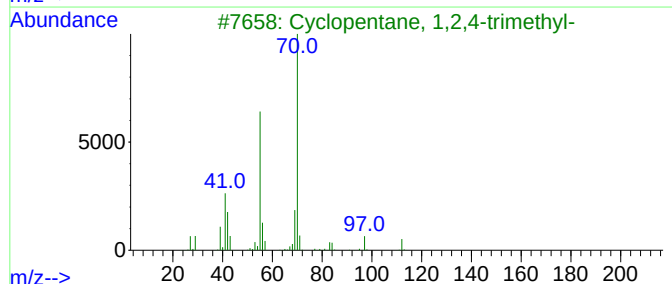
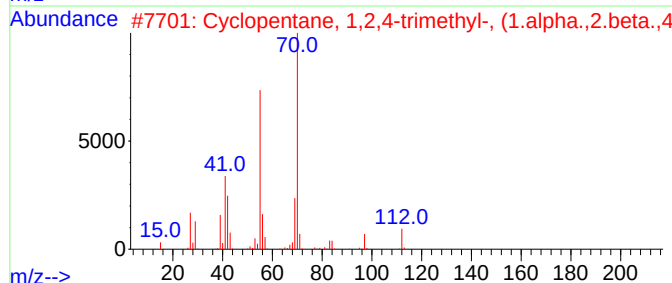
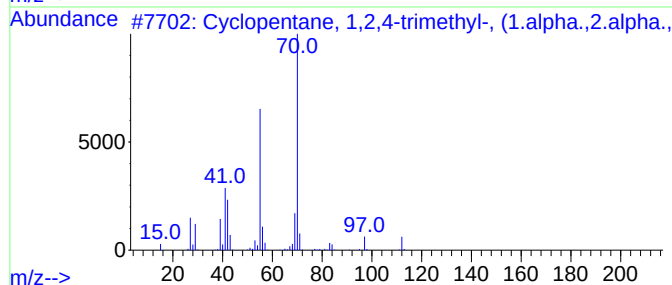
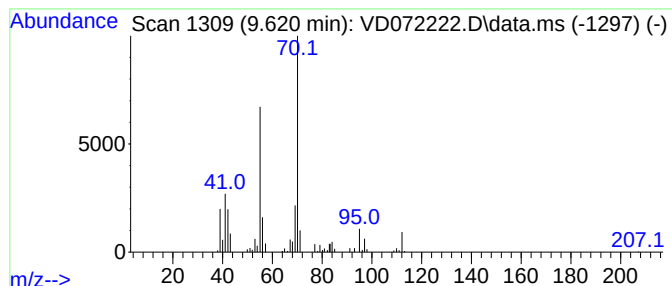
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031122S.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, 1,2,4-trimeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.620	7.31 ug/l	301468	1,4-Difluorobenzene	8.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	90
2			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	90
3			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	90
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	72
5			Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	72



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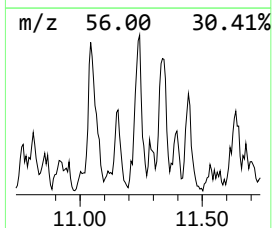
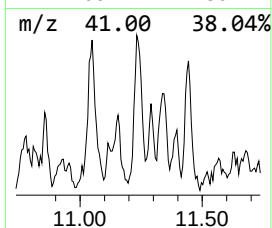
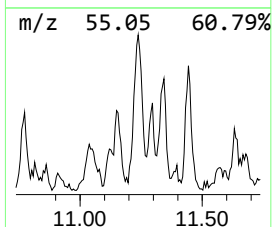
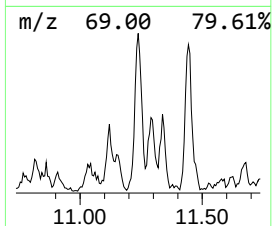
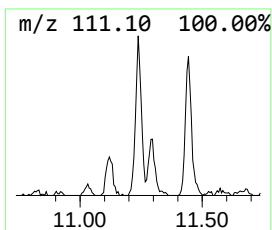
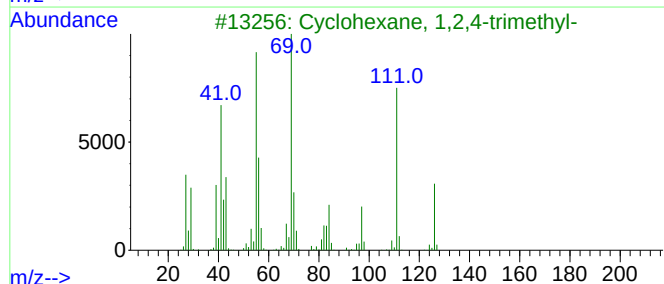
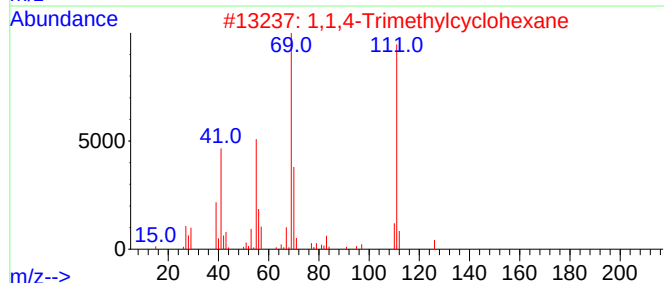
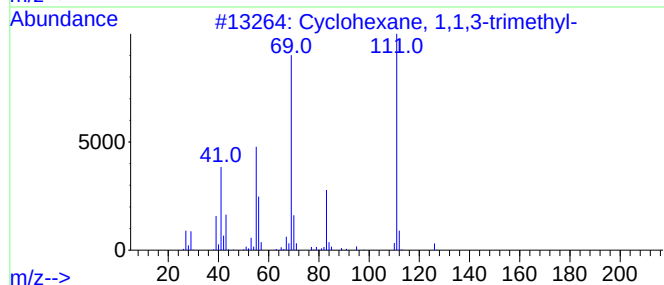
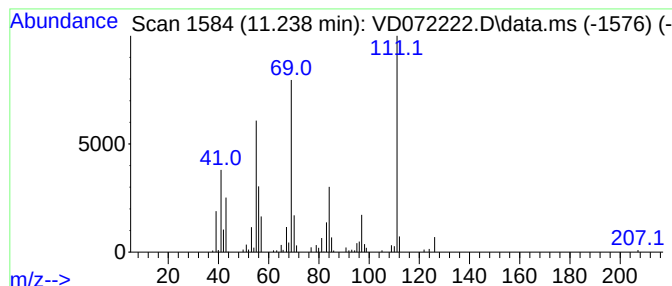
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D031122S.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.238	5.11 ug/l	291708	Chlorobenzene-d5	11.637

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	74
2			1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	64
3			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	64
4			2,3,4-Trimethyl-hex-3-enal	140	C9H16O	1000193-72-9	43
5			Cyclooctanemethanol	142	C9H18O	003637-63-6	43



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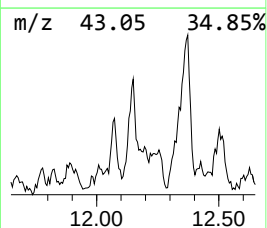
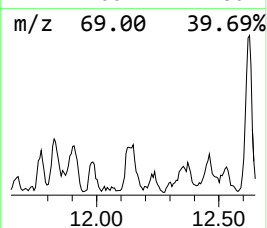
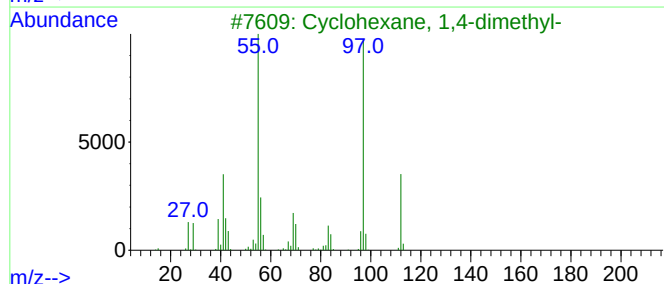
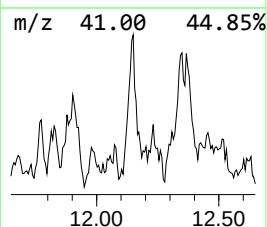
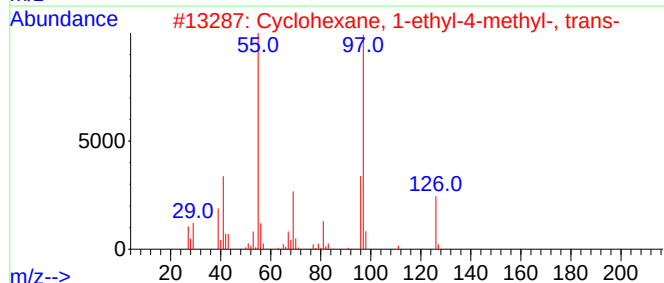
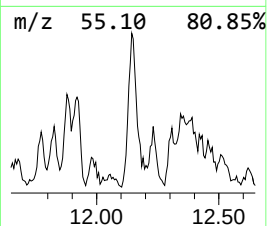
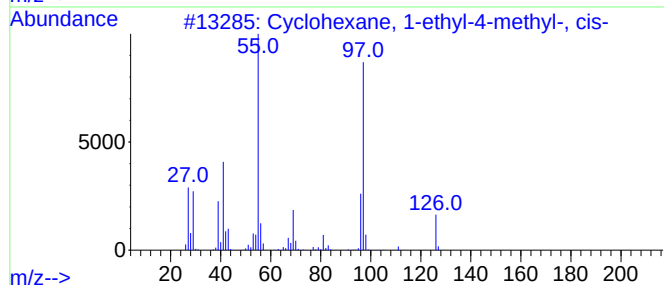
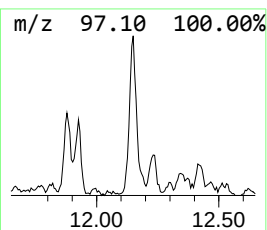
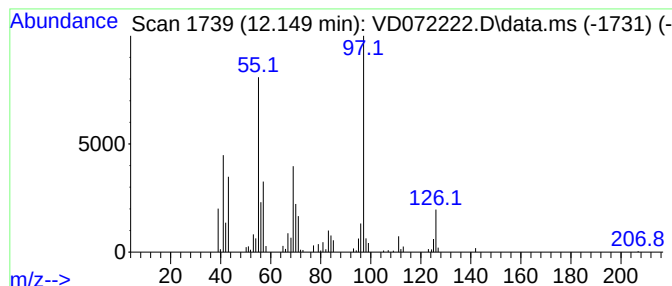
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.149	5.28 ug/l	301470	Chlorobenzene-d5	11.637

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	64
2			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	64
3			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	59
4			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	59
5			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	58



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.061	5.4	ug/l	178441	1	7.979	1641750	50.0
Cyclopentane, 1...	9.620	7.3	ug/l	301468	2	8.861	2062390	50.0
Cyclohexane, 1,...	11.238	5.1	ug/l	291708	3	11.637	2854500	50.0
Cyclohexane, 1-...	12.149	5.3	ug/l	301470	3	11.637	2854500	50.0