

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
 Data File : VY014644.D
 Acq On : 14 Jul 2023 13:52
 Operator : SY/MD
 Sample : 03601-01
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 HR-1-071223

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_Y\methods\82Y071323S.M
 Title : SW846 8260

Signal : TIC: VY014644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.704	460	473	487	rBV2	29365	97859	7.31%	0.873%
2	4.923	496	509	514	rBV2	4993	19354	1.45%	0.173%
3	5.734	633	642	652	rBV3	17456	55648	4.16%	0.496%
4	6.972	835	845	864	rBV	74907	234894	17.55%	2.096%
5	7.709	955	966	972	rBV	175348	417426	31.19%	3.724%
6	7.783	972	978	989	rVB	301153	672139	50.23%	5.996%
7	8.136	1024	1036	1050	rVB2	192965	454610	33.97%	4.056%
8	8.685	1118	1126	1139	rBV	460967	912419	68.18%	8.140%
9	9.179	1194	1207	1213	rBV2	33556	78932	5.90%	0.704%
10	9.459	1243	1253	1260	rVB6	6750	18834	1.41%	0.168%
11	9.605	1270	1277	1285	rVB2	10283	22514	1.68%	0.201%
12	9.758	1293	1302	1305	rBV2	10238	21745	1.62%	0.194%
13	9.819	1305	1312	1315	rBV3	12291	24633	1.84%	0.220%
14	9.953	1324	1334	1338	rBV4	18943	51626	3.86%	0.461%
15	10.172	1363	1370	1385	rVB	738170	1338191	100.00%	11.939%
16	10.361	1393	1401	1409	rVB3	26383	69791	5.22%	0.623%
17	10.514	1422	1426	1431	rVV	34358	59094	4.42%	0.527%
18	10.575	1431	1436	1440	rVV	34574	62441	4.67%	0.557%
19	10.617	1440	1443	1448	rVV3	17590	32028	2.39%	0.286%
20	10.709	1454	1458	1463	rVB	16552	24644	1.84%	0.220%
21	10.800	1467	1473	1479	rVB2	29577	52328	3.91%	0.467%
22	10.904	1483	1490	1492	rBV	23157	43093	3.22%	0.384%
23	10.940	1492	1496	1505	rVV	72950	161754	12.09%	1.443%
24	11.032	1507	1511	1515	rVV	46697	76057	5.68%	0.679%
25	11.087	1515	1520	1525	rVV	85701	142979	10.68%	1.276%
26	11.142	1525	1529	1533	rVV3	13693	20654	1.54%	0.184%
27	11.203	1533	1539	1543	rVV2	39673	71120	5.31%	0.634%
28	11.282	1543	1552	1562	rVB5	60435	193718	14.48%	1.728%
29	11.373	1562	1567	1572	rBV	46618	79411	5.93%	0.708%
30	11.483	1578	1585	1595	rBV	667820	1127349	84.24%	10.058%
31	11.575	1595	1600	1604	rBV5	8118	14539	1.09%	0.130%
32	11.623	1604	1608	1611	rBV3	15082	20469	1.53%	0.183%
33	11.672	1611	1616	1618	rBV3	22287	40473	3.02%	0.361%
34	11.709	1618	1622	1624	rBV2	37128	51059	3.82%	0.456%
35	11.843	1638	1644	1646	rBV5	8247	16468	1.23%	0.147%
36	11.898	1646	1653	1654	rVV2	11542	22699	1.70%	0.203%

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Integrator: RTE

Smoothing : ON

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Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	11.928	1654	1658	1662	rVB2	19857	32687	2.44%	0.292%
38	12.001	1662	1670	1677	rBV4	70077	190548	14.24%	1.700%
39	12.087	1681	1684	1685	rVV2	12198	13907	1.04%	0.124%
40	12.117	1685	1689	1693	rVB2	56271	80768	6.04%	0.721%
41	12.202	1697	1703	1705	rVV3	49495	93501	6.99%	0.834%
42	12.233	1705	1708	1714	rVB2	75811	135041	10.09%	1.205%
43	12.373	1725	1731	1735	rBV6	23673	55677	4.16%	0.497%
44	12.410	1735	1737	1743	rVB4	25168	39894	2.98%	0.356%
45	12.477	1743	1748	1754	rBV	566728	868087	64.87%	7.745%
46	12.519	1754	1755	1759	rVB3	20821	15954	1.19%	0.142%
47	12.568	1759	1763	1767	rVB4	9444	15959	1.19%	0.142%
48	12.641	1770	1775	1782	rVB4	54599	104305	7.79%	0.931%
49	12.727	1782	1789	1793	rBV3	45958	95879	7.16%	0.855%
50	12.806	1793	1802	1807	rBV6	106258	203922	15.24%	1.819%
51	13.038	1836	1840	1847	rVB2	64222	100294	7.49%	0.895%
52	13.117	1847	1853	1858	rBV2	50024	81089	6.06%	0.723%
53	13.166	1858	1861	1866	rBV6	12803	21534	1.61%	0.192%
54	13.214	1866	1869	1872	rBV2	13399	17831	1.33%	0.159%
55	13.312	1877	1885	1889	rBV6	47456	97129	7.26%	0.867%
56	13.361	1889	1893	1896	rVV4	23687	35735	2.67%	0.319%
57	13.422	1896	1903	1912	rVB	685410	1114776	83.30%	9.945%
58	13.495	1912	1915	1922	rVB4	14183	22082	1.65%	0.197%
59	13.562	1922	1926	1931	rBV3	18586	39796	2.97%	0.355%
60	13.617	1933	1935	1938	rVB2	15270	16904	1.26%	0.151%
61	13.660	1938	1942	1950	rVB2	26186	45446	3.40%	0.405%
62	13.745	1950	1956	1961	rBV4	52069	97484	7.28%	0.870%
63	13.818	1961	1968	1972	rBV2	23171	50097	3.74%	0.447%
64	13.909	1980	1983	1988	rVB5	22978	31551	2.36%	0.281%
65	13.964	1989	1992	1997	rVB2	37309	55118	4.12%	0.492%
66	14.013	1997	2000	2005	rVB5	12158	18157	1.36%	0.162%
67	14.074	2005	2010	2015	rBV3	31982	54101	4.04%	0.483%
68	14.141	2015	2021	2026	rVB6	15417	36979	2.76%	0.330%
69	14.208	2027	2032	2035	rBV2	18510	34999	2.62%	0.312%
70	14.257	2035	2040	2044	rBV7	19576	36652	2.74%	0.327%
71	14.330	2050	2052	2056	rVB	20813	24858	1.86%	0.222%
72	14.373	2056	2059	2063	rBV4	16997	24091	1.80%	0.215%
73	14.415	2063	2066	2071	rVB3	20089	26892	2.01%	0.240%
74	14.611	2095	2098	2101	rVB	14262	16816	1.26%	0.150%
75	14.672	2102	2108	2114	rVV3	40721	98710	7.38%	0.881%
76	14.732	2115	2118	2124	rVB4	17604	28157	2.10%	0.251%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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77	14.940	2147	2152	2155	rBV5	16490	25367	1.90%	0.226%
78	15.049	2165	2170	2176	rVB3	14879	28367	2.12%	0.253%
79	15.208	2190	2196	2205	rVB7	11171	37288	2.79%	0.333%
80	15.312	2206	2213	2221	rBV3	23566	61119	4.57%	0.545%
81	15.604	2257	2261	2266	rVB8	8750	13751	1.03%	0.123%
82	16.031	2324	2331	2338	rVB8	9575	18052	1.35%	0.161%
83	16.287	2368	2373	2377	rBV2	10779	17061	1.27%	0.152%
84	16.482	2399	2405	2413	rBV3	13564	31557	2.36%	0.282%

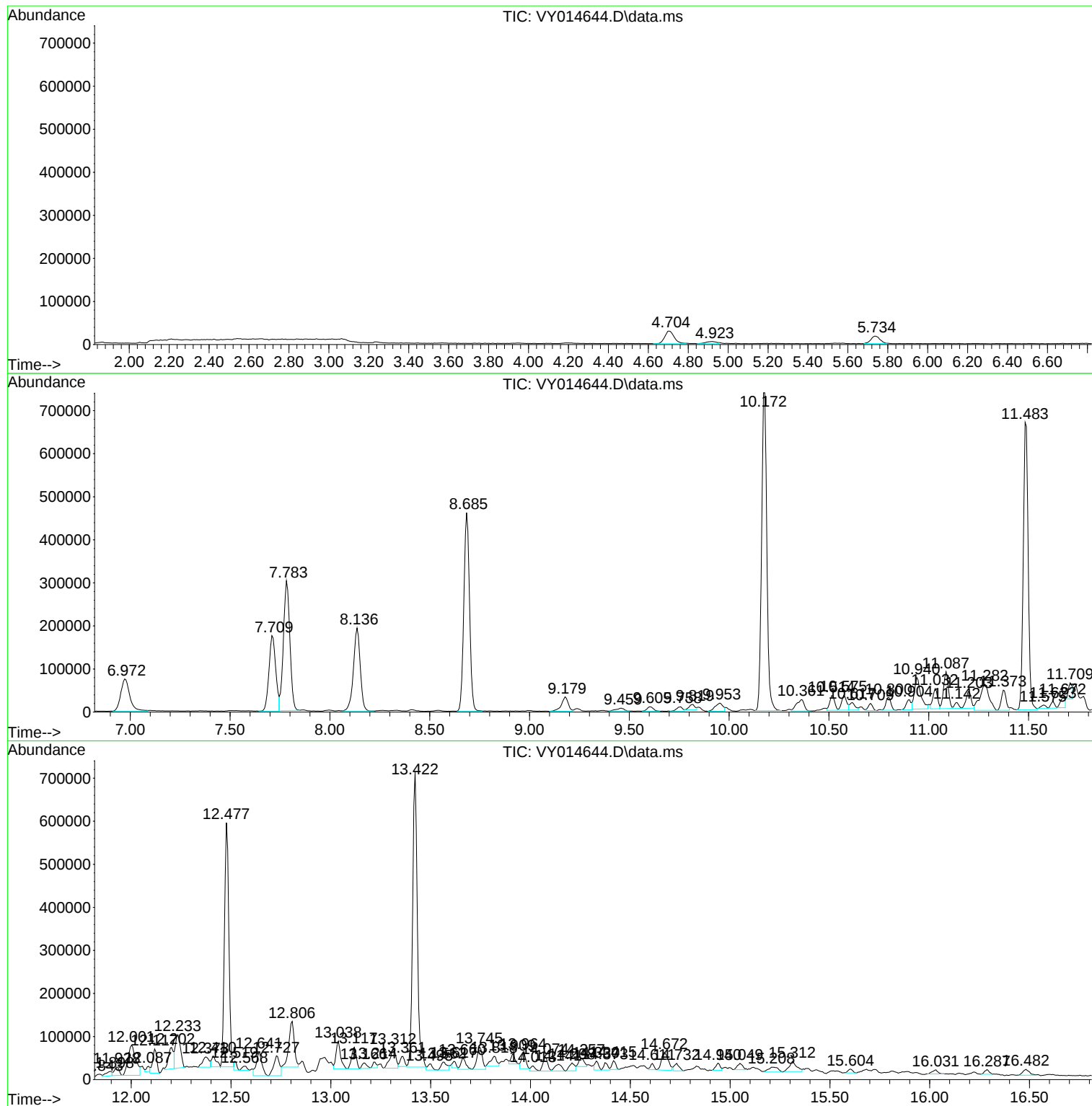
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-1-071223

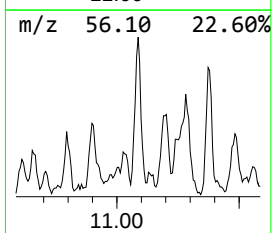
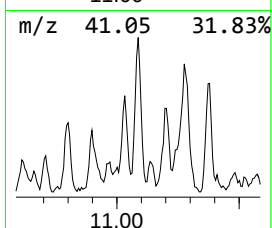
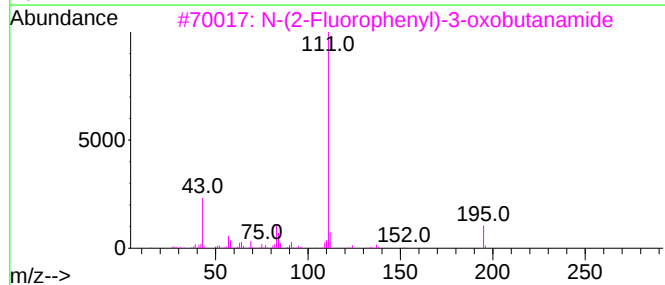
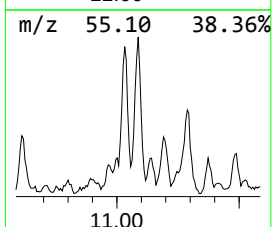
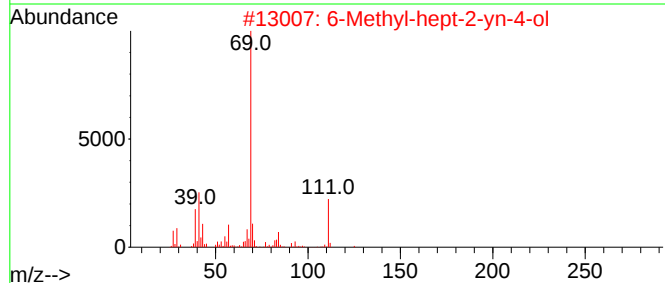
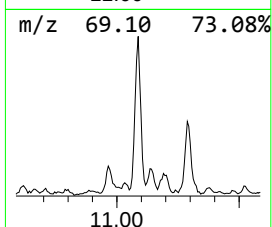
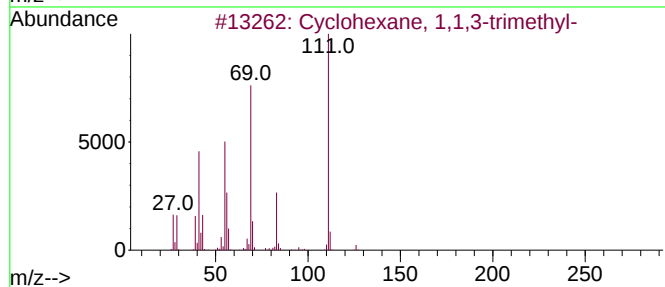
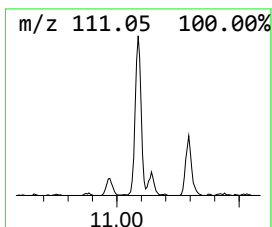
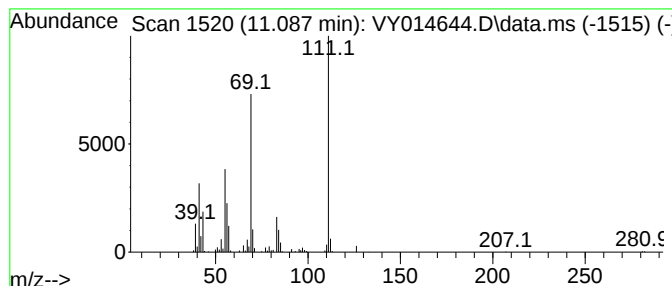
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.087	6.34 ug/l	142979	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	64
2			6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	59
3			N-(2-Fluorophenyl)-3-oxobutanamide	195	C10H10FNO2	1000486-19-7	59
4			p-Fluoroaniline	111	C6H6FN	000371-40-4	58
5			3'-Fluoroacetanilide	153	C8H8FNO	000351-28-0	53



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Operator : SY/MD
Sample : 03601-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

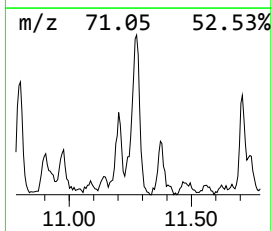
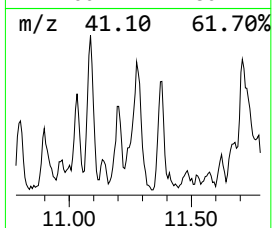
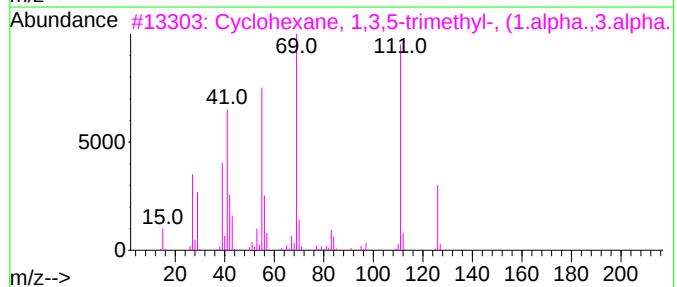
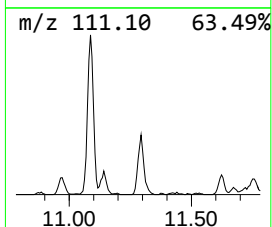
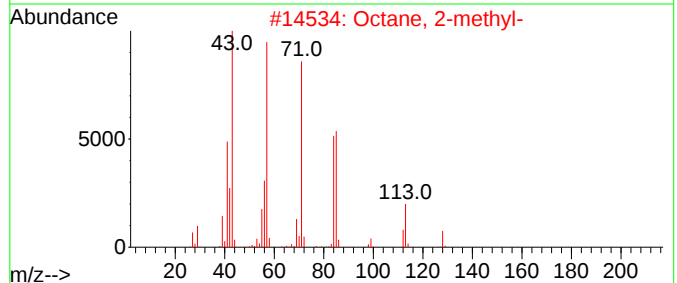
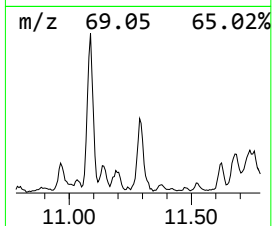
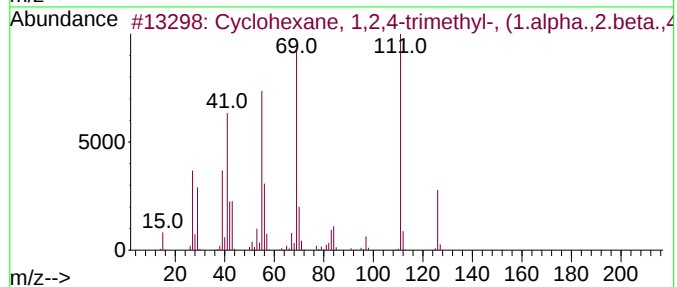
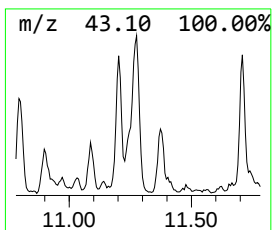
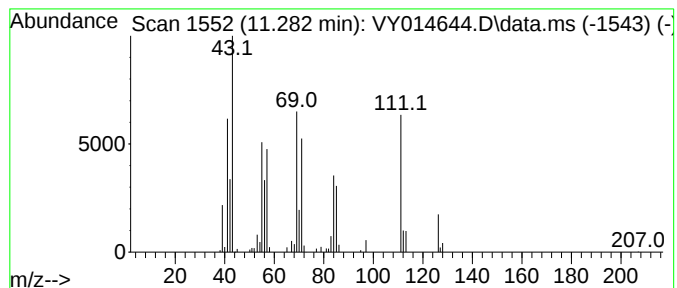
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,2,4-trimethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.282	8.59 ug/l	193718	Chlorobenzene-d5			11.489
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...)		126	C9H18	007667-60-9	50
2	Octane, 2-methyl-		128	C9H20	003221-61-2	46
3	Cyclohexane, 1,3,5-trimethyl-, (...)		126	C9H18	001795-26-2	38
4	Cyclohexane, 1,2,4-trimethyl-		126	C9H18	002234-75-5	38
5	Cyclohexane, 1,3,5-trimethyl-		126	C9H18	001839-63-0	30



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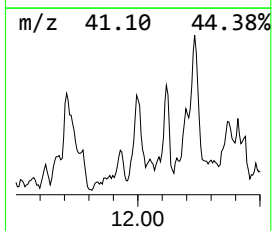
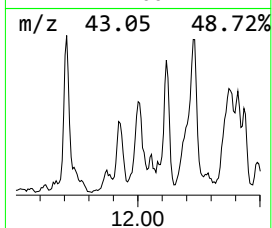
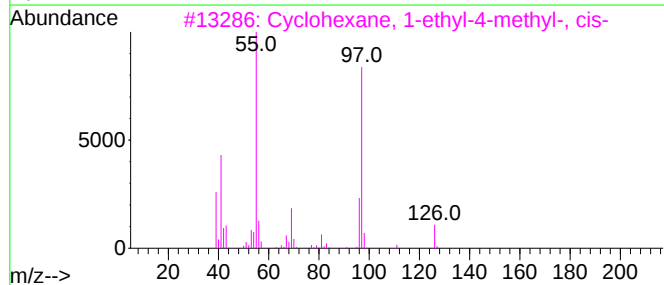
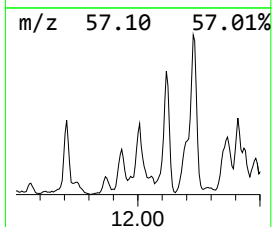
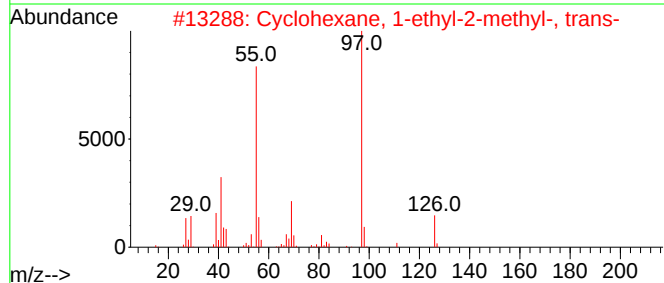
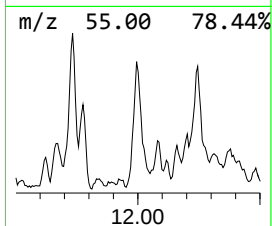
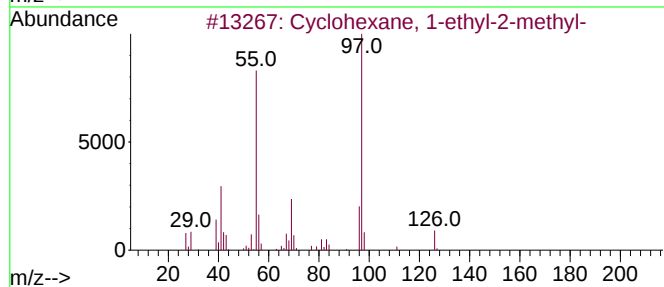
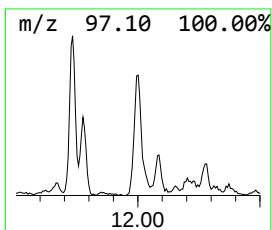
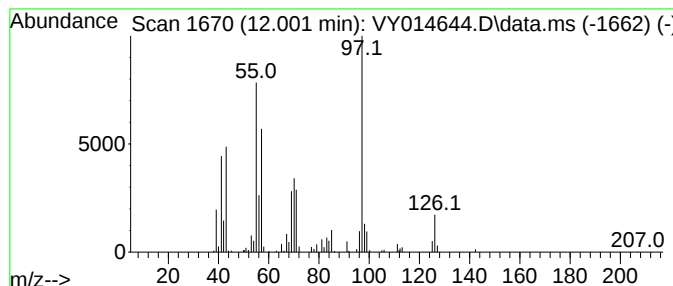
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.001	8.45 ug/l	190548	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	64
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	60
4			Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	59
5			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52



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HR-1-071223

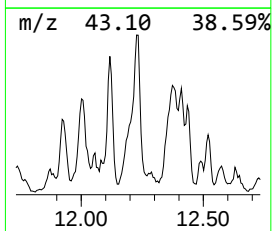
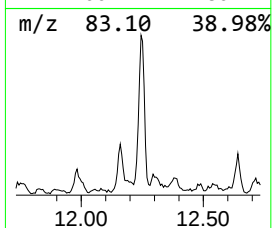
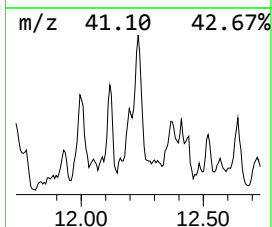
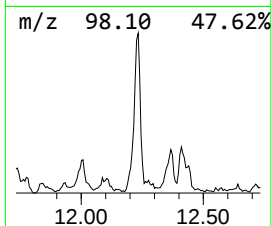
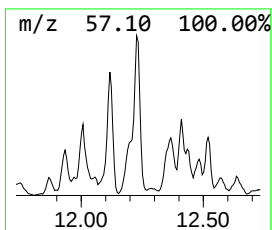
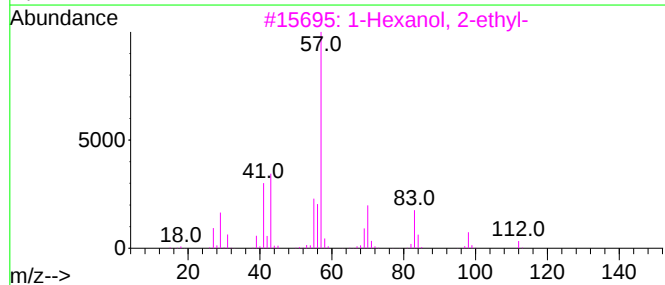
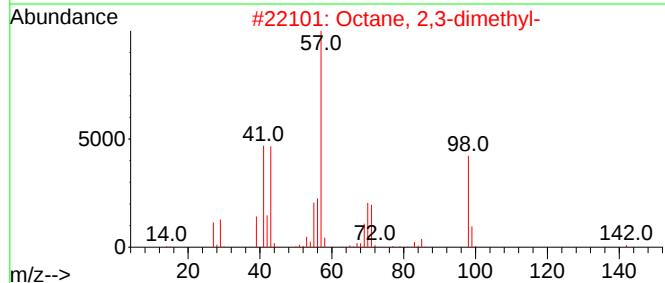
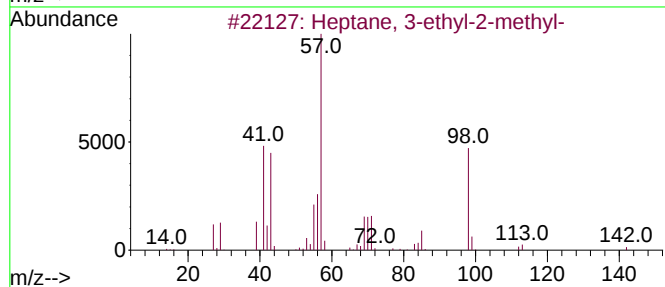
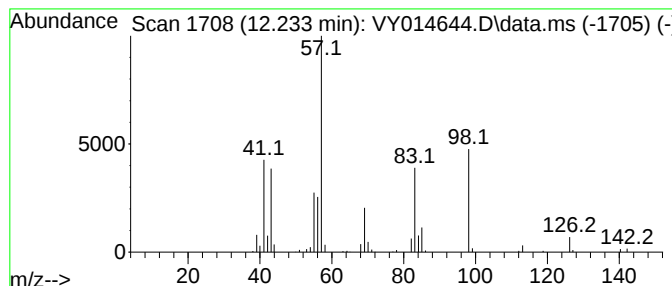
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Quant Title : SW846 8260

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

Peak Number 7 Heptane, 3-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	5.99 ug/l	135041	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	50
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	40
4			Ether, tert-butyl isopropylidene...	154	C10H18O	024524-56-9	25
5			Dodecyl heptyl ether	284	C19H40O	1010406-39-2	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071423\
Data File : VY014644.D
Acq On : 14 Jul 2023 13:52
Operator : SY/MD
Sample : 03601-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
HR-1-071223

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1,...	11.087	6.3	ug/l	142979	3	11.489	1127350	50.0
Cyclohexane, 1,...	11.282	8.6	ug/l	193718	3	11.489	1127350	50.0
Cyclohexane, 1-...	12.001	8.4	ug/l	190548	3	11.489	1127350	50.0
Heptane, 3-ethy...	12.233	6.0	ug/l	135041	3	11.489	1127350	50.0