

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
 Data File : VY012247.D
 Acq On : 18 Jan 2023 15:40
 Operator : KP/MD
 Sample : 01179-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 VNJ-208

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\82Y011623S.M
 Title : SW846 8260

Signal : TIC: VY012247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.247	63	70	78	rVB	14000	23004	1.87%	0.274%
2	3.942	337	348	368	rBV	152497	420539	34.15%	5.011%
3	4.716	465	475	488	rBV4	9586	29583	2.40%	0.352%
4	6.972	831	845	863	rBV	25401	81276	6.60%	0.968%
5	7.716	957	967	972	rBV2	91502	211225	17.15%	2.517%
6	7.789	972	979	991	rVB	179793	418804	34.00%	4.990%
7	8.136	1023	1036	1047	rBV2	80716	208093	16.90%	2.479%
8	8.685	1116	1126	1140	rBV	254888	511527	41.53%	6.095%
9	9.179	1197	1207	1213	rBV3	27708	58820	4.78%	0.701%
10	9.758	1296	1302	1306	rBV	7424	14272	1.16%	0.170%
11	9.819	1306	1312	1316	rBV	48835	92576	7.52%	1.103%
12	9.959	1326	1335	1347	rVB	52304	113201	9.19%	1.349%
13	10.179	1363	1371	1386	rBV	509254	937762	76.14%	11.174%
14	10.368	1393	1402	1409	rVB	107432	182597	14.83%	2.176%
15	10.520	1411	1427	1432	rBV	42552	79186	6.43%	0.944%
16	10.575	1432	1436	1439	rVV	29379	51579	4.19%	0.615%
17	10.618	1439	1443	1448	rVV	57319	103145	8.37%	1.229%
18	10.709	1454	1458	1463	rVB	13313	19579	1.59%	0.233%
19	10.801	1467	1473	1479	rVB	23450	36971	3.00%	0.441%
20	10.904	1483	1490	1492	rBV	22698	37203	3.02%	0.443%
21	10.971	1492	1501	1504	rVV2	47176	133678	10.85%	1.593%
22	11.002	1504	1506	1508	rVV	36289	46857	3.80%	0.558%
23	11.032	1508	1511	1516	rVV	67408	112365	9.12%	1.339%
24	11.087	1516	1520	1526	rVV	34515	59016	4.79%	0.703%
25	11.203	1533	1539	1543	rBV3	22293	38175	3.10%	0.455%
26	11.282	1543	1552	1563	rVB4	90096	263196	21.37%	3.136%
27	11.380	1563	1568	1573	rBV	59995	88453	7.18%	1.054%
28	11.490	1579	1586	1596	rBV	355365	572469	46.48%	6.821%
29	11.593	1596	1603	1606	rBV	104608	171927	13.96%	2.049%
30	11.697	1612	1620	1631	rBV	558662	1231623	100.00%	14.675%
31	11.782	1631	1634	1640	rVB	23183	34446	2.80%	0.410%
32	12.026	1663	1674	1682	rBV	229321	415410	33.73%	4.950%
33	12.203	1699	1703	1706	rVV4	9916	16125	1.31%	0.192%
34	12.252	1706	1711	1719	rVB4	14159	28402	2.31%	0.338%
35	12.483	1742	1749	1760	rVB2	273873	460227	37.37%	5.484%
36	12.733	1784	1790	1794	rVV	7715	12841	1.04%	0.153%

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Integrator: RTE

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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

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37	12.806	1797	1802	1809	rVB5	18677	35951	2.92%	0.428%
38	12.965	1822	1828	1837	rVB7	5627	14772	1.20%	0.176%
39	13.117	1846	1853	1859	rBV	14828	27237	2.21%	0.325%
40	13.422	1897	1903	1912	rVB	307051	482541	39.18%	5.750%
41	13.623	1932	1936	1940	rBV3	8074	13376	1.09%	0.159%
42	13.666	1940	1943	1952	rVB5	7359	16131	1.31%	0.192%
43	13.751	1952	1957	1961	rBV	26550	40467	3.29%	0.482%
44	13.965	1988	1992	1997	rVB3	11080	18147	1.47%	0.216%
45	14.257	2033	2040	2045	rBV9	5826	13198	1.07%	0.157%
46	14.611	2093	2098	2103	rVB2	36127	50436	4.10%	0.601%
47	14.678	2103	2109	2114	rBV5	14745	32835	2.67%	0.391%
48	14.727	2114	2117	2125	rVB5	10644	20609	1.67%	0.246%
49	14.837	2127	2135	2143	rBV3	9865	20752	1.68%	0.247%
50	15.050	2164	2170	2176	rBV4	10020	20909	1.70%	0.249%
51	15.135	2180	2184	2190	rVB8	6204	13113	1.06%	0.156%
52	15.312	2206	2213	2217	rBV3	14618	35661	2.90%	0.425%
53	15.434	2229	2233	2241	rVB3	26701	42864	3.48%	0.511%
54	15.525	2242	2248	2255	rBV5	7036	16520	1.34%	0.197%
55	15.727	2276	2281	2289	rVB2	21891	38914	3.16%	0.464%
56	16.031	2325	2331	2336	rBV4	10282	22311	1.81%	0.266%
57	16.227	2356	2363	2369	rBV4	13964	28168	2.29%	0.336%
58	16.294	2369	2374	2380	rVV	15239	30433	2.47%	0.363%
59	16.361	2380	2385	2393	rVB4	7819	15367	1.25%	0.183%
60	16.495	2400	2407	2412	rBV3	10324	25743	2.09%	0.307%

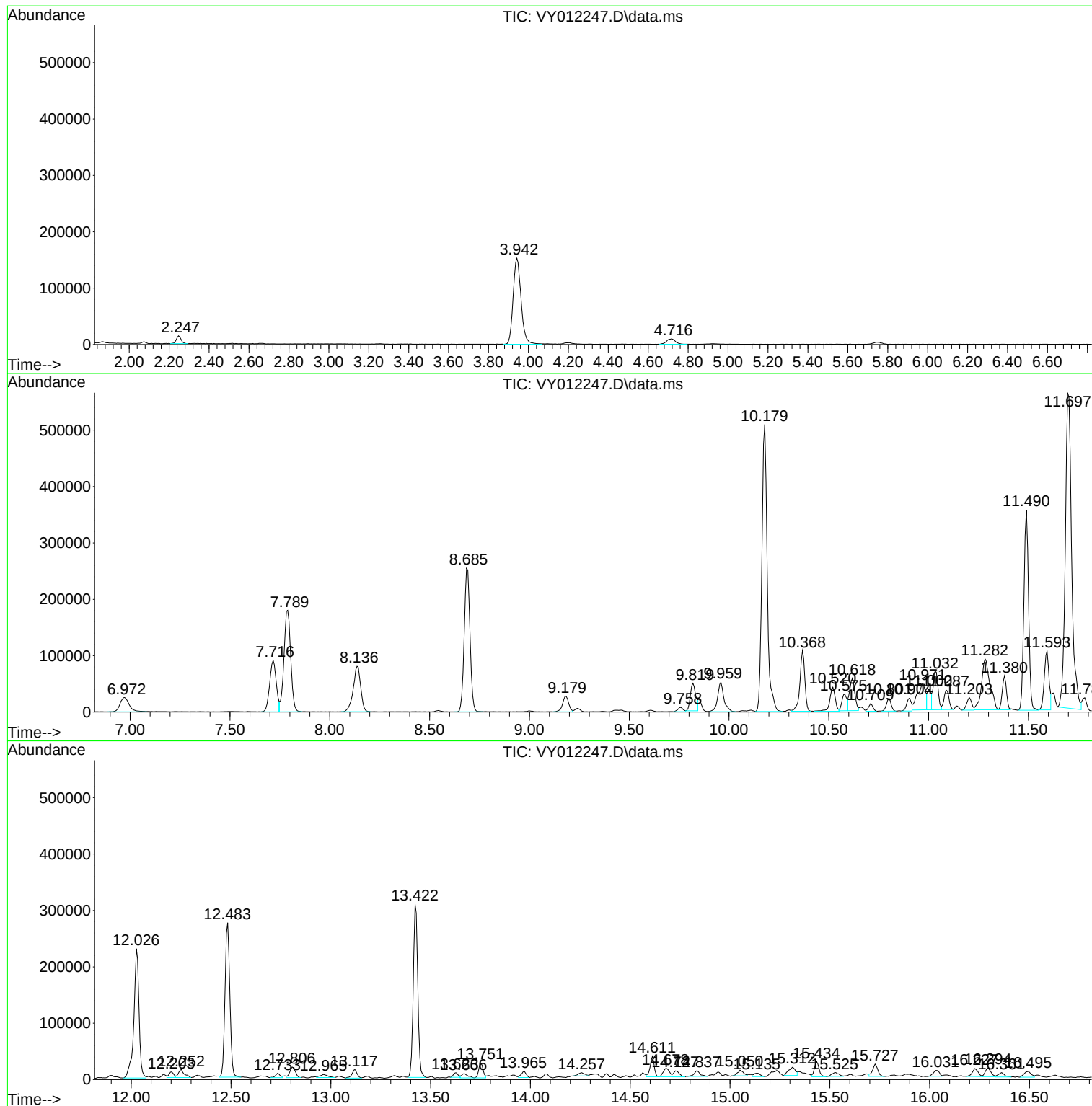
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Quant Title : SW846 8260

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



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

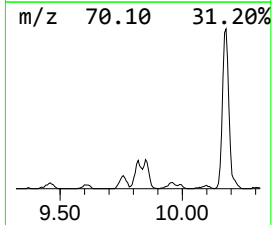
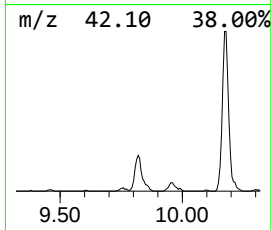
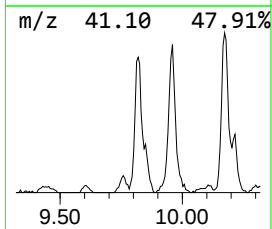
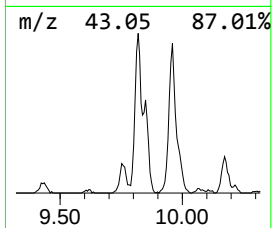
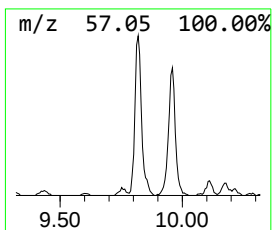
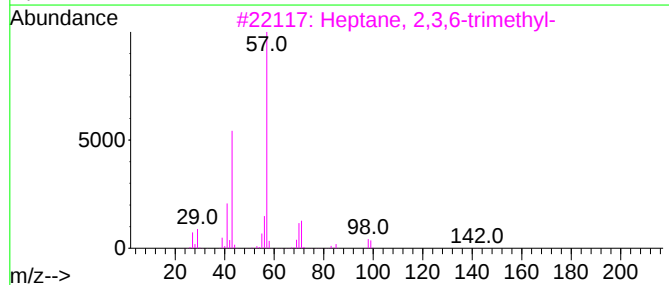
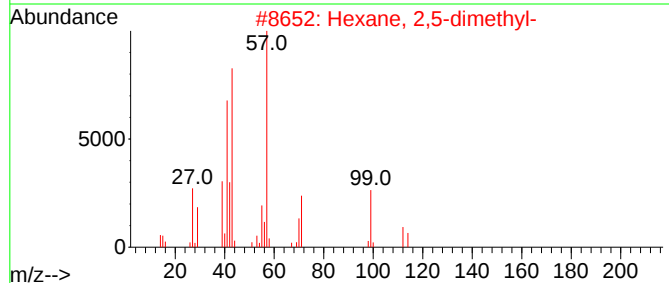
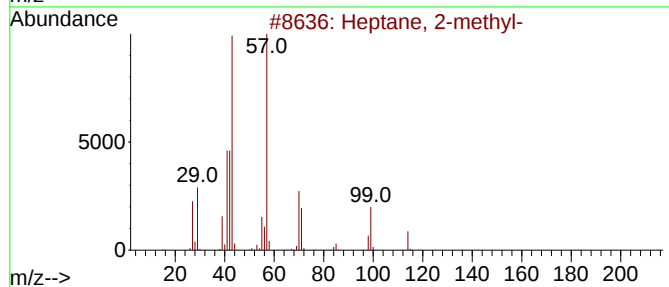
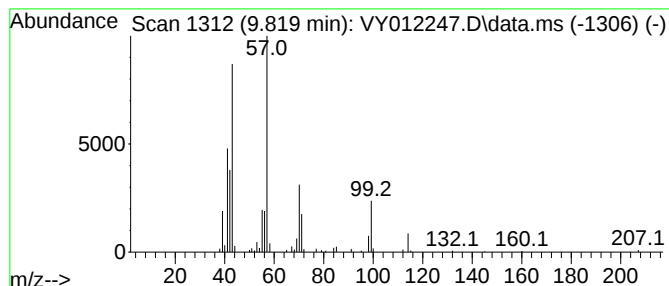
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.819	9.05 ug/l	92576	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	95
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	87
3			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	43
4			Heptane, 3-ethyl-	128	C9H20	015869-80-4	43
5			1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	40



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Misc : 5.01g/5.0mL/MSVOA_Y/soil
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

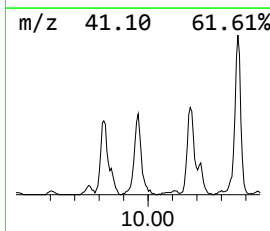
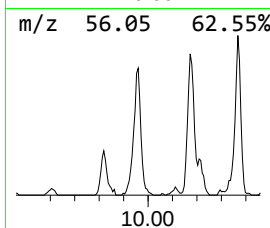
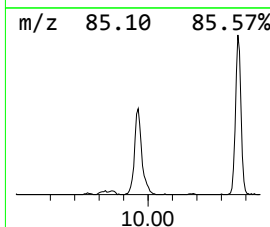
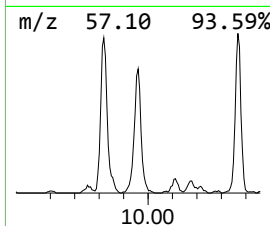
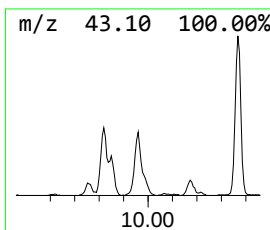
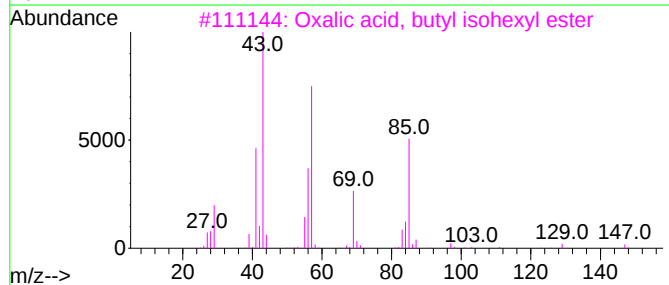
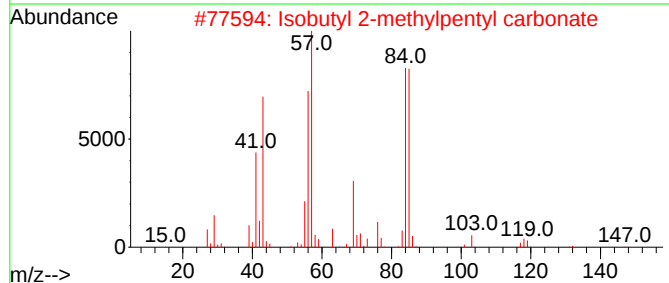
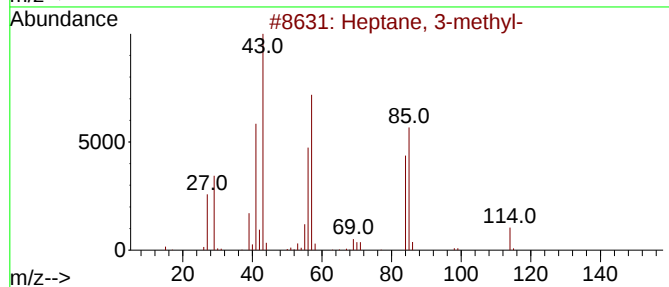
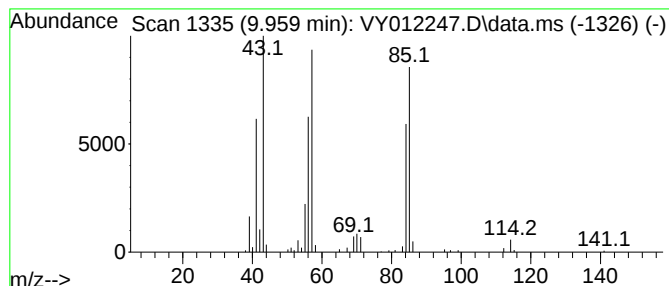
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.959	11.07 ug/l	113201	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Isobutyl 2-methylpentyl carbonate	202	C11H22O3	1000372-75-2	72
3			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	72
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53
5			Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
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Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-208

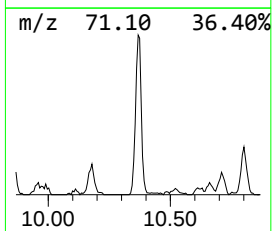
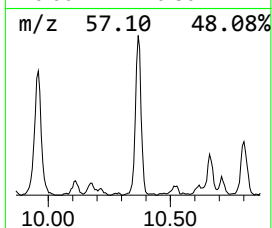
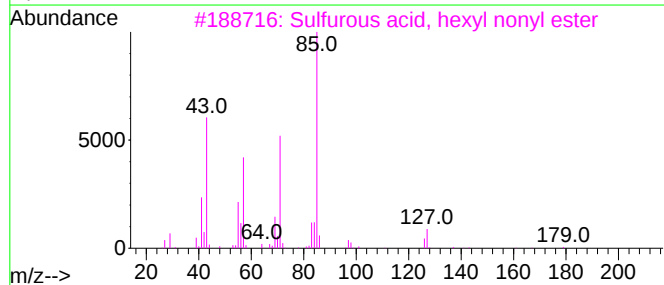
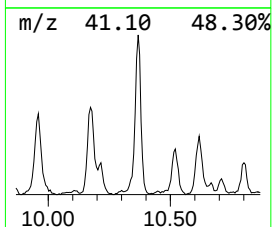
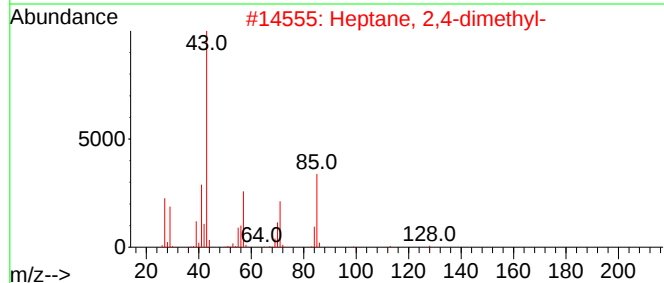
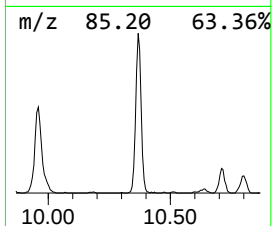
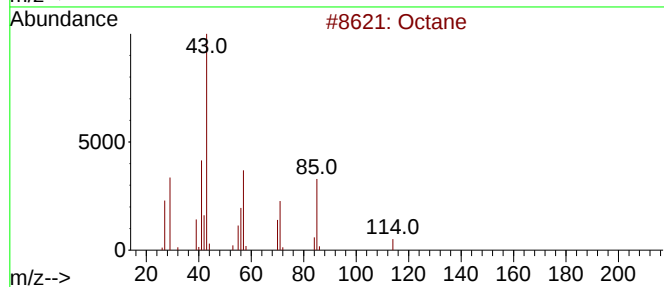
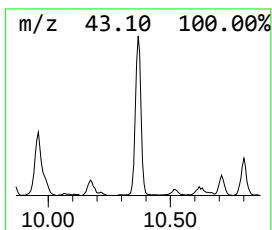
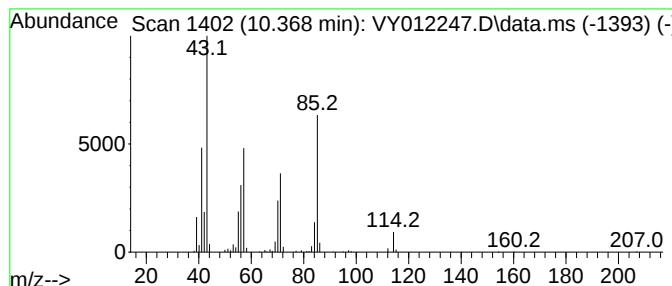
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	15.95 ug/l	182597	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	94
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
3			Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	59
4			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	59
5			Heptane, 4,4-dimethyl-	128	C9H20	001068-19-5	50



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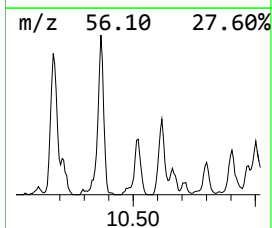
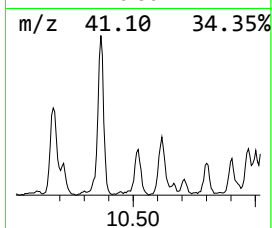
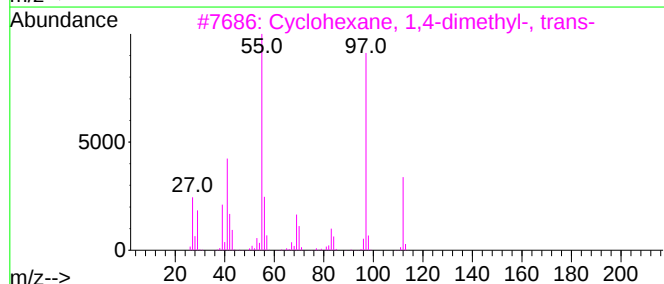
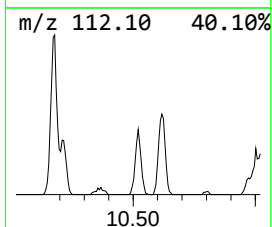
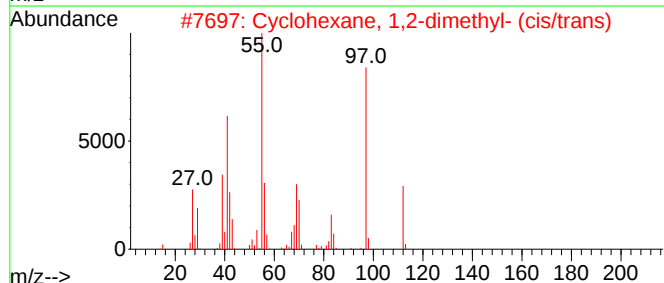
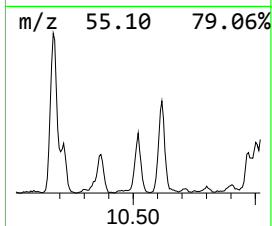
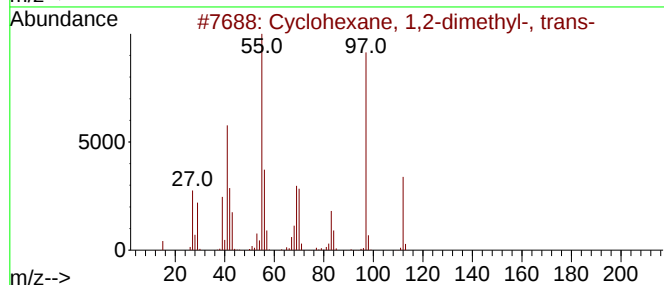
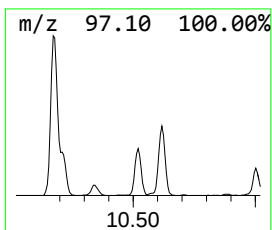
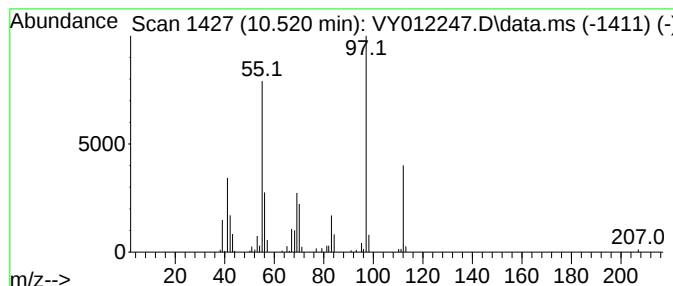
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.520	6.92 ug/l	79186	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	95
2			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	94
3			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	87
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
5			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	87



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VNJ-208

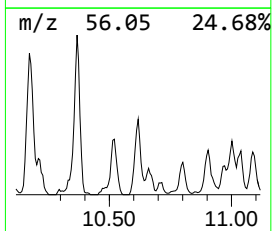
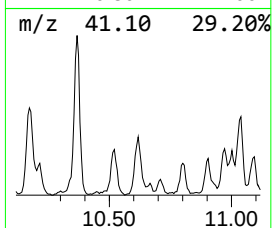
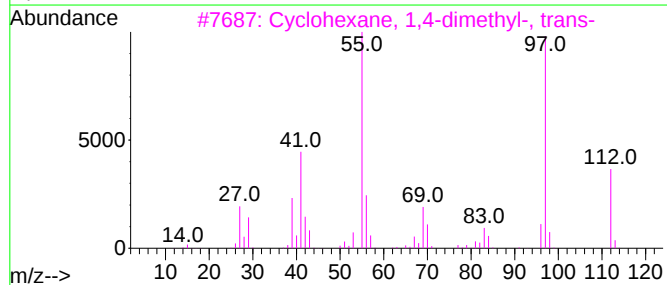
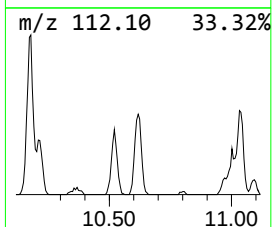
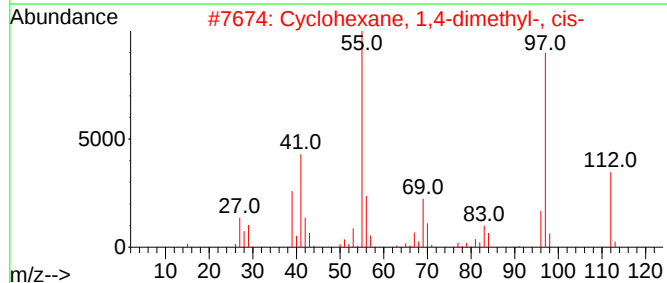
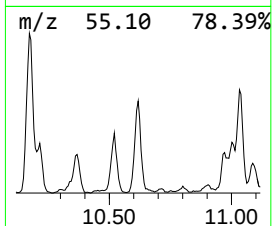
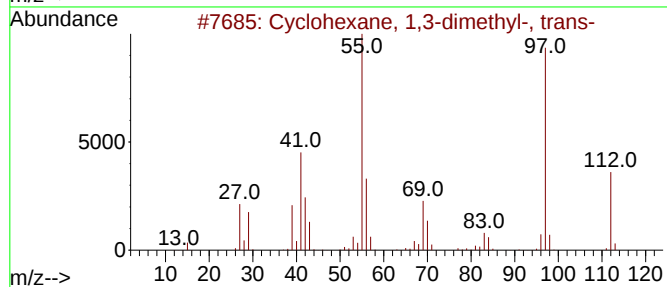
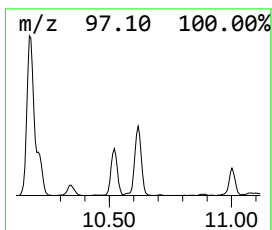
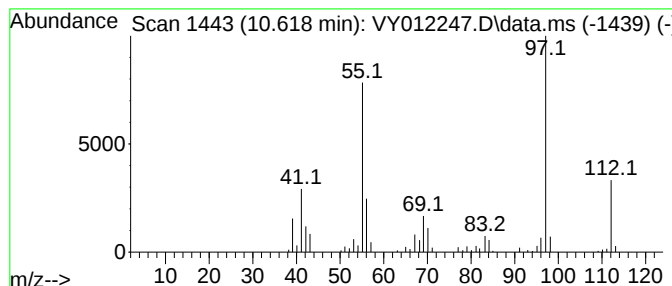
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.618	9.01 ug/l	103145	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	94
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	94
3			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	91
4			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87
5			Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
Data File : VY012247.D
Acq On : 18 Jan 2023 15:40
Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

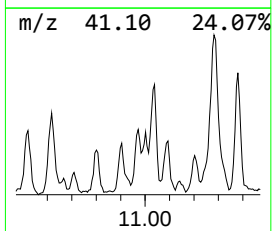
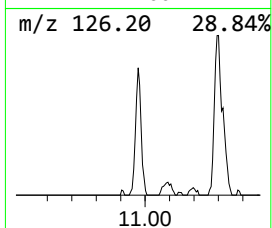
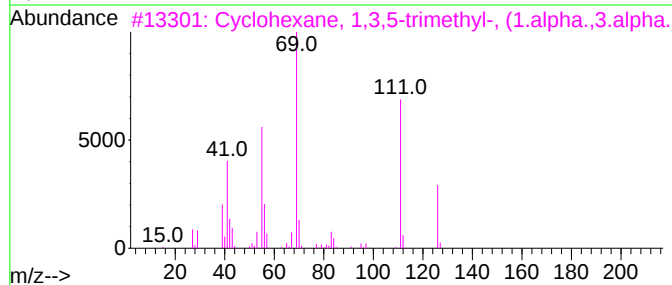
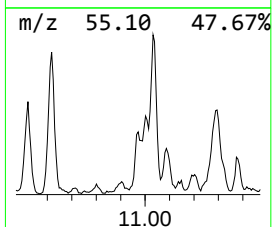
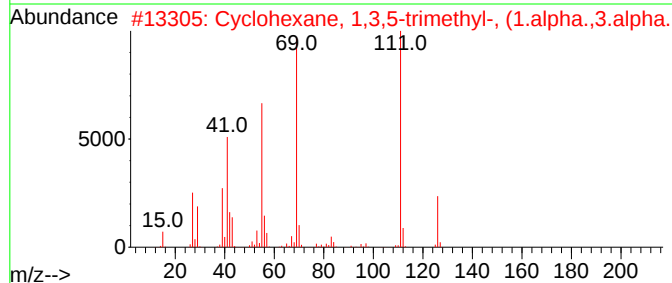
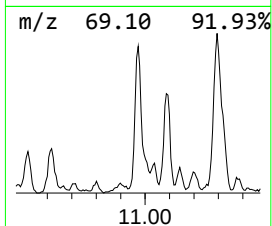
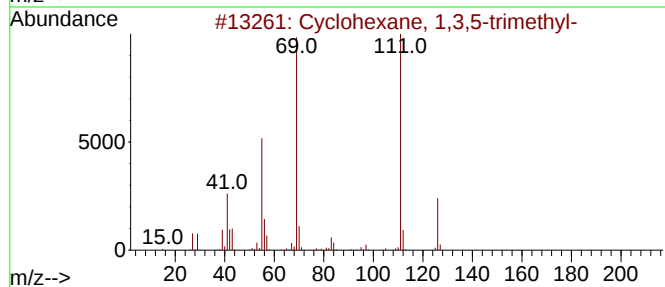
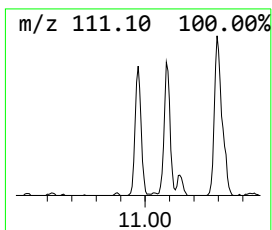
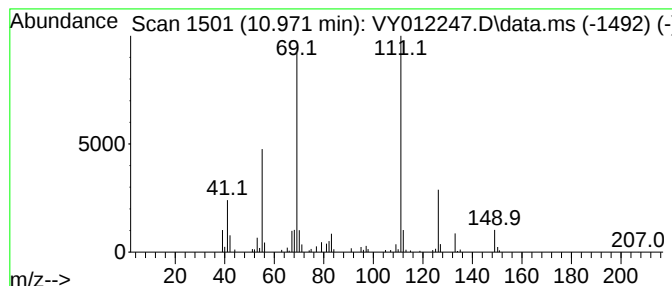
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.971	11.68 ug/l	133678	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	91
2			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	87
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	83
4			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	72
5			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
Data File : VY012247.D
Acq On : 18 Jan 2023 15:40
Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/soil
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

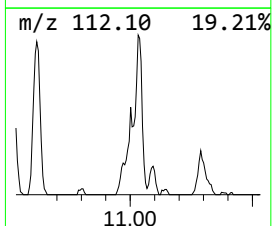
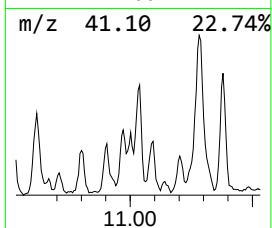
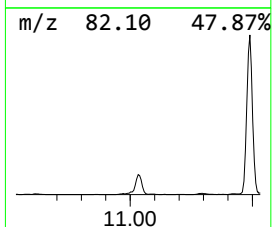
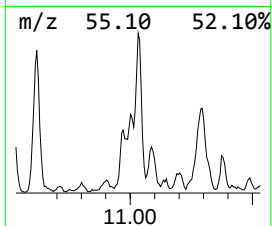
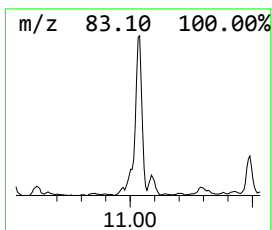
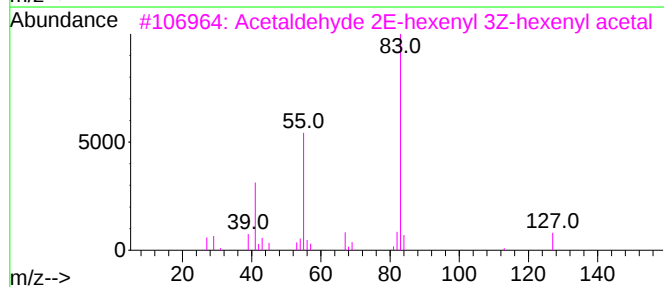
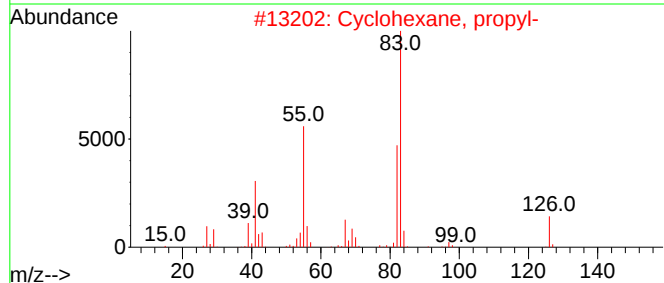
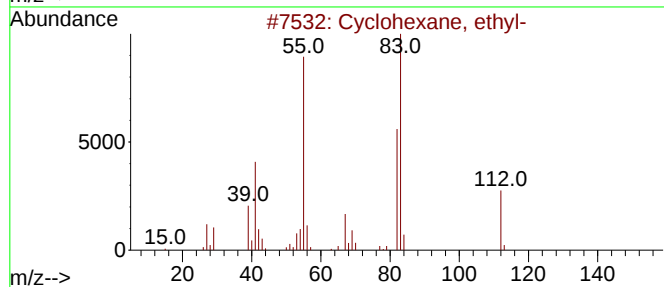
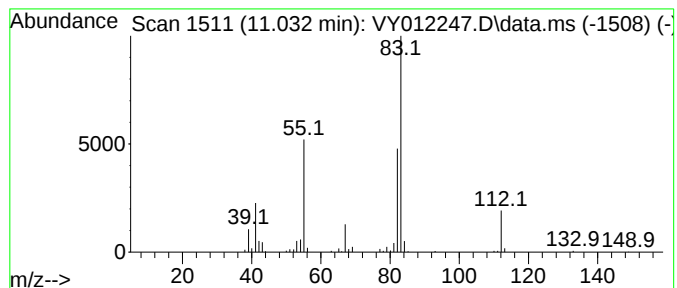
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.032	9.81 ug/l	112365	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethyl-	112	C8H16	001678-91-7	91
2			Cyclohexane, propyl-	126	C9H18	001678-92-8	64
3			Acetaldehyde 2E-hexenyl 3Z-hexen...	226	C14H26O2	1000431-45-5	50
4			Oxalic acid, cyclohexyl propyl e...	214	C11H18O4	1000309-30-3	50
5			4-Oxohex-2-enal	112	C6H8O2	020697-55-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
Data File : VY012247.D
Acq On : 18 Jan 2023 15:40
Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

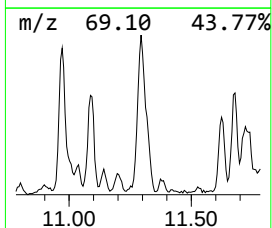
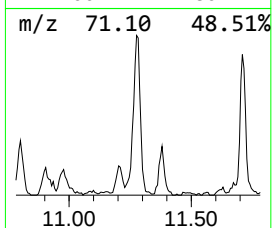
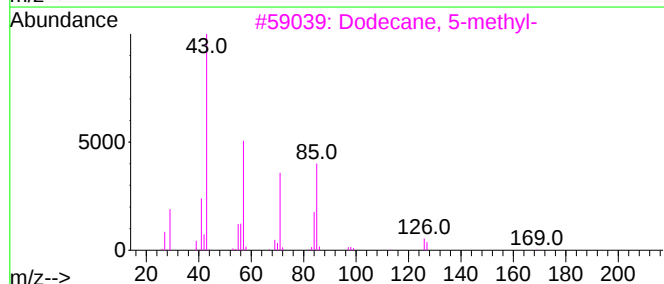
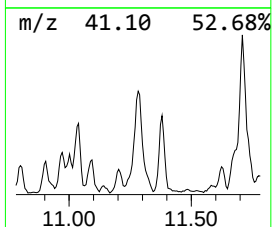
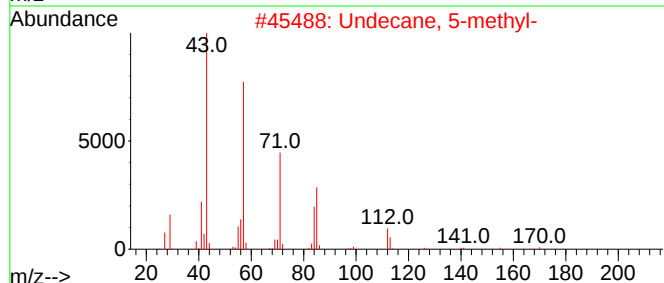
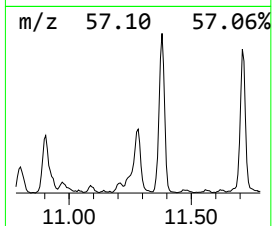
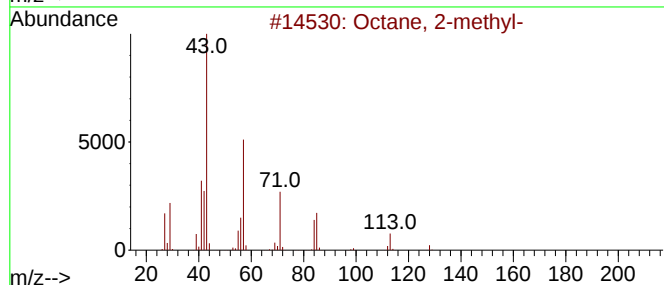
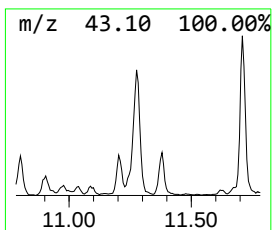
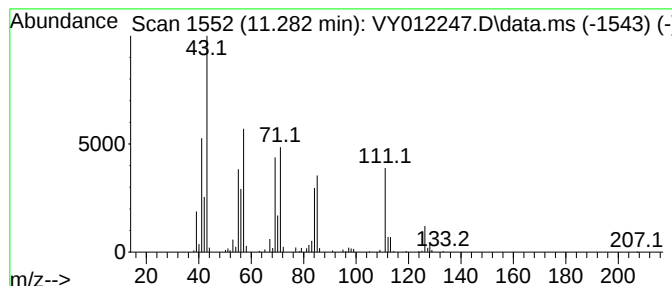
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Quant Title : SW846 8260

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

Peak Number 9 unknown11.282 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	22.99 ug/l	263196	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-		128	C9H20		003221-61-2	43
2	Undecane, 5-methyl-		170	C12H26		001632-70-8	35
3	Dodecane, 5-methyl-		184	C13H28		017453-93-9	35
4	1-Butanol, 2,3-dimethyl-		102	C6H14O		019550-30-2	27
5	Heptane, 2,4-dimethyl-		128	C9H20		002213-23-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
Data File : VY012247.D
Acq On : 18 Jan 2023 15:40
Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

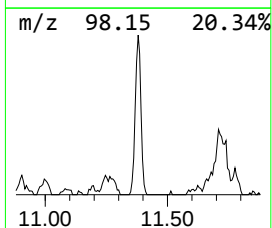
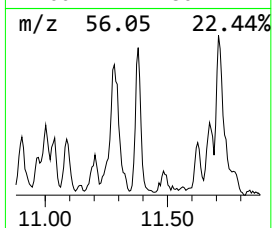
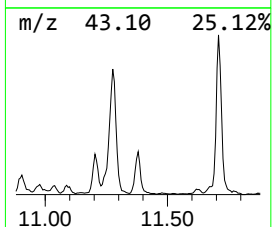
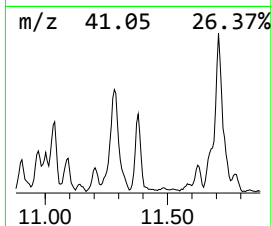
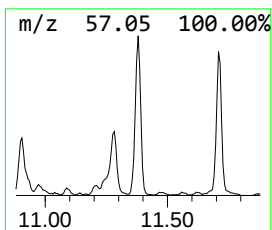
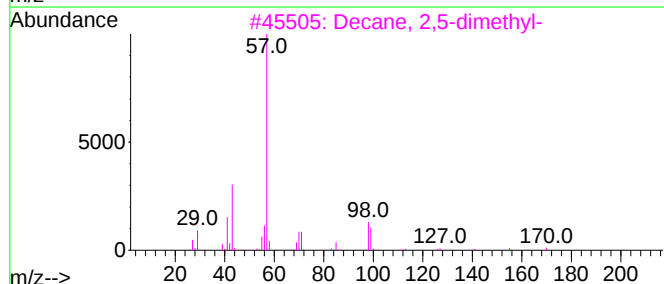
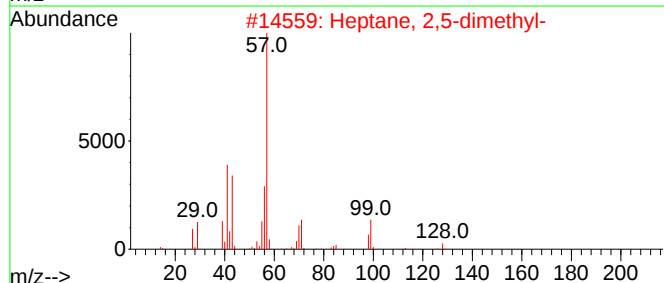
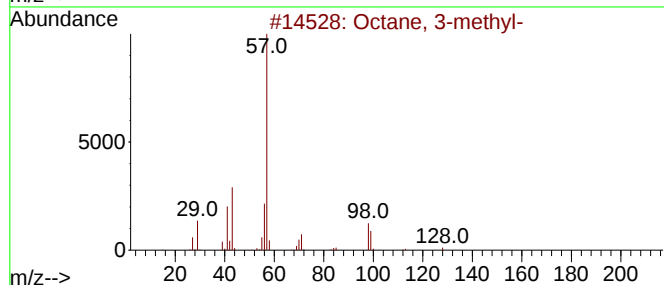
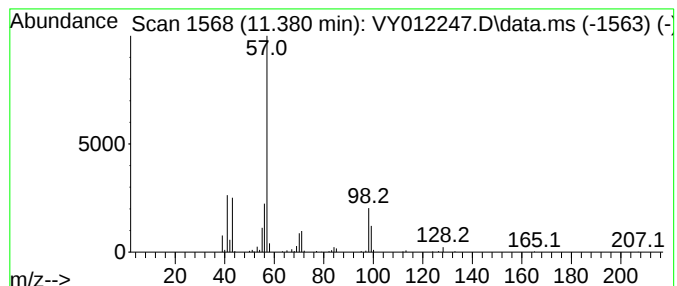
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Quant Title : SW846 8260

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

Peak Number 10 Octane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	7.73 ug/l	88453	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3-methyl-	128	C9H20	002216-33-3	91
2			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	81
3			Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	59
4			Undecane, 6-methyl-	170	C12H26	017302-33-9	45
5			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011823\
Data File : VY012247.D
Acq On : 18 Jan 2023 15:40
Operator : KP/MD
Sample : 01179-01
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
VNJ-208

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011623S.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
Heptane, 2-methyl-	9.819	9.1	ug/l	92576	2	8.691	511527	50.0
Heptane, 3-methyl-	9.959	11.1	ug/l	113201	2	8.691	511527	50.0
Octane	10.368	15.9	ug/l	182597	3	11.490	572469	50.0
Cyclohexane, 1,...	10.520	6.9	ug/l	79186	3	11.490	572469	50.0
Cyclohexane, 1,...	10.618	9.0	ug/l	103145	3	11.490	572469	50.0
Cyclohexane, 1,...	10.971	11.7	ug/l	133678	3	11.490	572469	50.0
Cyclohexane, et...	11.032	9.8	ug/l	112365	3	11.490	572469	50.0
unknown11.282	11.282	23.0	ug/l	263196	3	11.490	572469	50.0
Octane, 3-methyl-	11.380	7.7	ug/l	88453	3	11.490	572469	50.0