

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051122\
 Data File : VY008716.D
 Acq On : 11 May 2022 18:47
 Operator : KP/MD
 Sample : N2781-06
 Misc : 5.33g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 P003-SS004-0006-01

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\82Y050922S.M
 Title : SW846 8260

Signal : TIC: VY008716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.027	353	362	372	rVB2	6639	17406	1.34%	0.223%
2	4.704	463	473	488	rVB2	7483	24615	1.90%	0.315%
3	5.747	634	644	653	rBV3	5011	15227	1.18%	0.195%
4	7.716	957	967	972	rBV	139098	329385	25.42%	4.213%
5	7.783	972	978	991	rVB	228585	529321	40.85%	6.770%
6	8.136	1021	1036	1049	rBV2	166287	527671	40.72%	6.749%
7	8.685	1118	1126	1135	rBV	341225	673230	51.95%	8.611%
8	9.746	1294	1300	1306	rBV3	7710	17193	1.33%	0.220%
9	10.179	1364	1371	1379	rVV	544292	912580	70.42%	11.672%
10	10.264	1379	1385	1387	rVV2	30909	54369	4.20%	0.695%
11	10.288	1387	1389	1395	rVB3	38166	51953	4.01%	0.664%
12	10.374	1395	1403	1408	rBV4	11460	22848	1.76%	0.292%
13	10.575	1428	1436	1443	rVV	71861	137499	10.61%	1.759%
14	10.959	1492	1499	1508	rBV4	7925	20340	1.57%	0.260%
15	11.319	1552	1558	1563	rVB2	11340	18989	1.47%	0.243%
16	11.489	1576	1586	1593	rBV	488101	808648	62.40%	10.343%
17	11.563	1593	1598	1602	rVV	15682	23328	1.80%	0.298%
18	11.746	1622	1628	1634	rVB	28371	45780	3.53%	0.586%
19	11.941	1655	1660	1663	rBV	17261	27269	2.10%	0.349%
20	12.111	1682	1688	1698	rVB	43186	75894	5.86%	0.971%
21	12.337	1722	1725	1728	rVV	8839	13235	1.02%	0.169%
22	12.471	1739	1747	1756	rBV3	509636	1295904	100.00%	16.575%
23	12.556	1756	1761	1768	rBV2	38663	89744	6.93%	1.148%
24	12.623	1768	1772	1783	rVB	89228	199476	15.39%	2.551%
25	12.831	1796	1806	1812	rBV3	63121	165483	12.77%	2.117%
26	12.886	1812	1815	1823	rVB2	21798	35459	2.74%	0.454%
27	12.983	1823	1831	1834	rBV5	12289	27952	2.16%	0.358%
28	13.068	1836	1845	1857	rVB	126440	243683	18.80%	3.117%
29	13.178	1857	1863	1870	rVB	42877	67893	5.24%	0.868%
30	13.282	1870	1880	1886	rBV	162096	284541	21.96%	3.639%
31	13.349	1886	1891	1895	rVV6	13160	30888	2.38%	0.395%
32	13.428	1895	1904	1908	rVV	419913	707136	54.57%	9.044%
33	13.483	1908	1913	1923	rVB	105888	233633	18.03%	2.988%
34	13.642	1932	1939	1947	rBV2	34237	63140	4.87%	0.808%
35	13.965	1986	1992	2006	rVB3	11195	26924	2.08%	0.344%

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P003-SS004-0006-01

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\82Y050922S.M
Title : SW846 8260

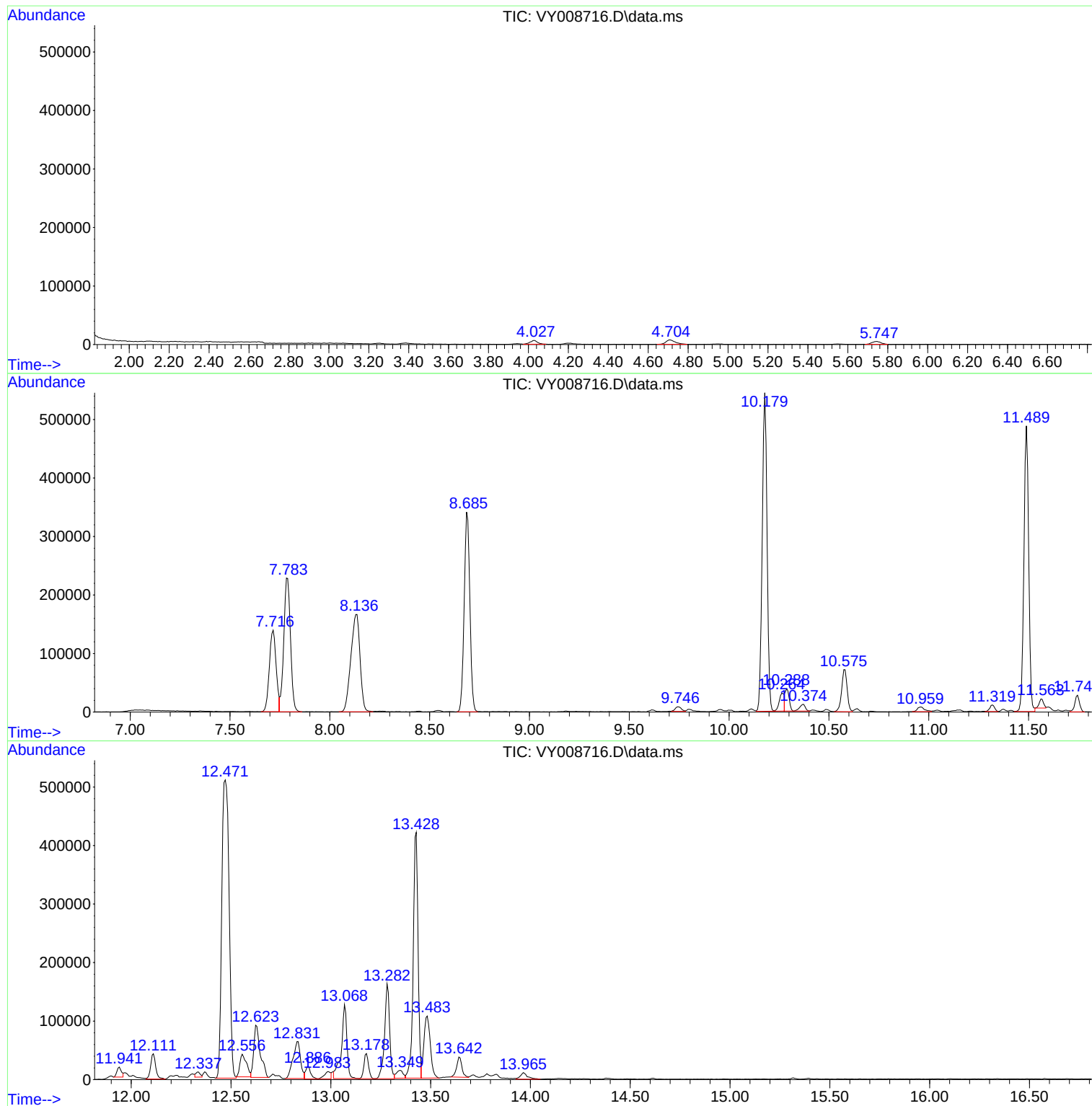
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050922S.M
Quant Title : SW846 8260

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



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Instrument :
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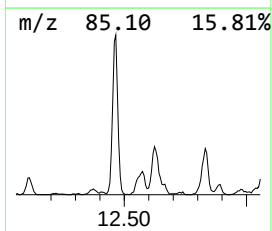
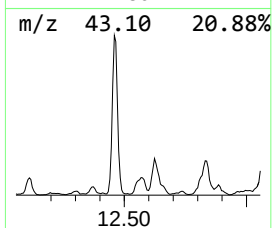
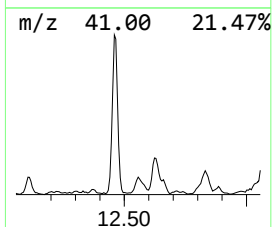
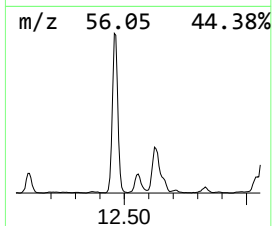
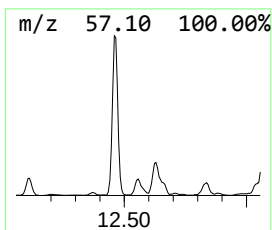
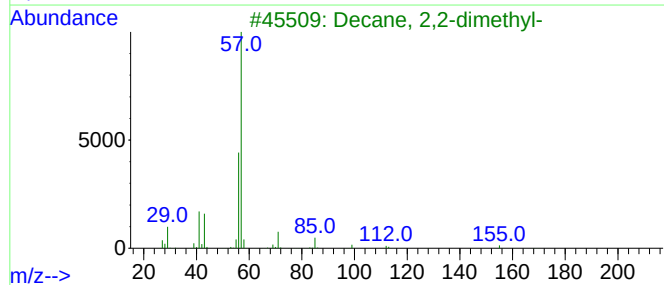
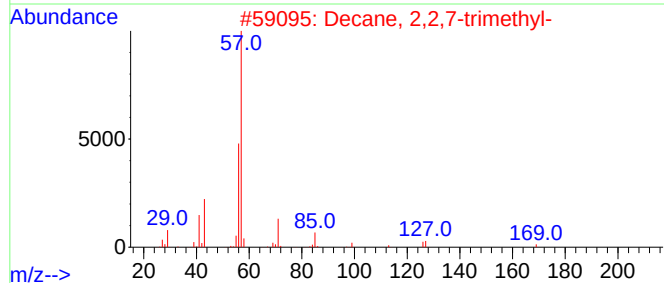
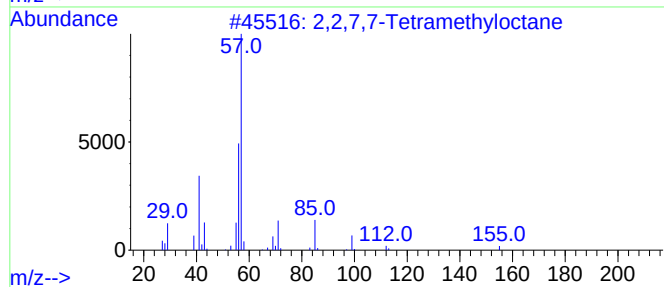
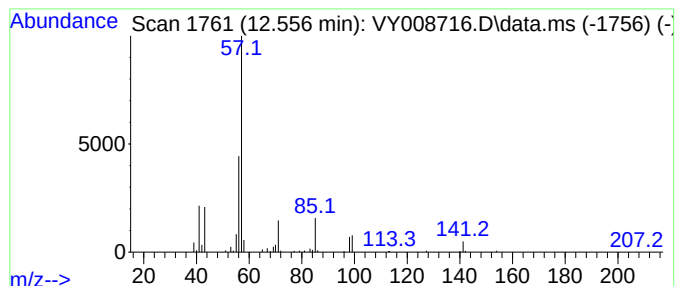
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Quant Title : SW846 8260

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

Peak Number 2 2,2,7,7-Tetramethyloctane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.556	6.35 ug/l	89744	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	72
2			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	72
3			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	72
4			Decane, 2,2,4-trimethyl-	184	C13H28	062237-98-3	64
5			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	64



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
P003-SS004-0006-01

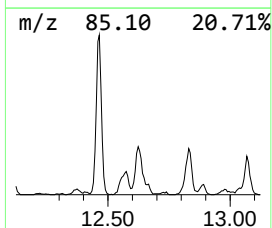
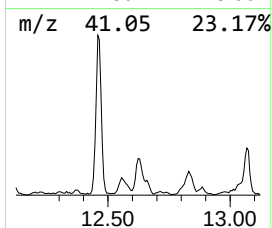
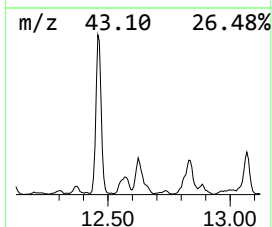
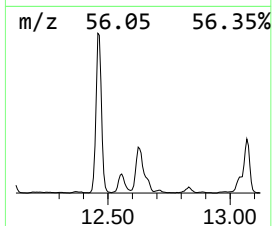
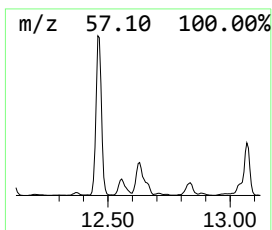
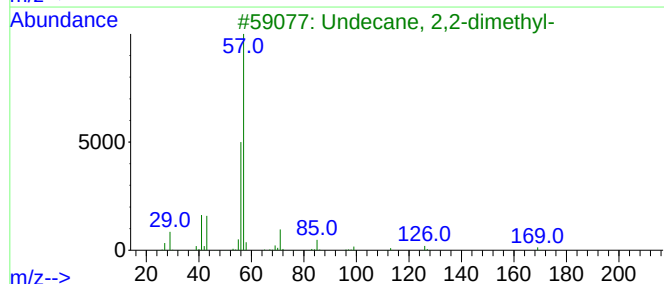
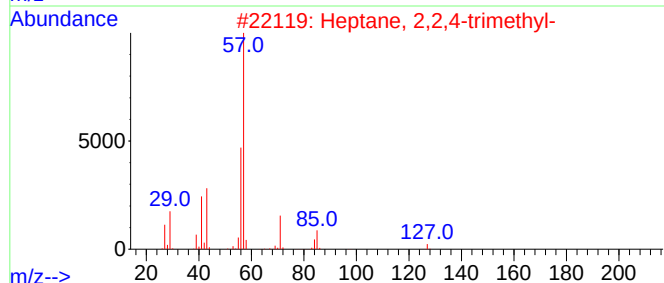
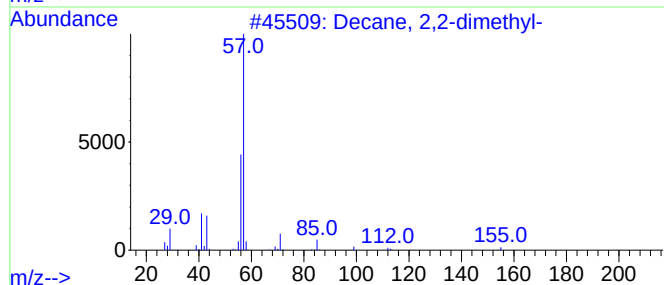
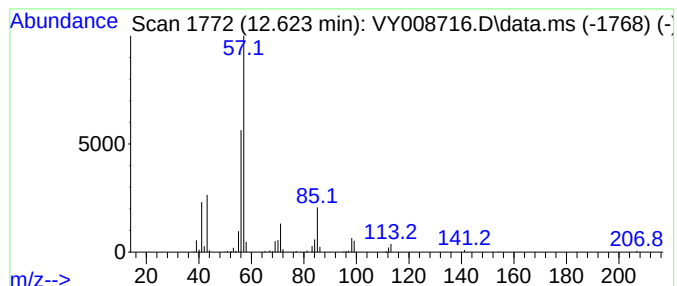
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Quant Title : SW846 8260

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

Peak Number 3 Decane, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.623	14.10 ug/l	199476	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	59
2			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	53
3			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	53
4			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	53
5			trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47



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Instrument :
MSVOA_Y
ClientSampleId :
P003-SS004-0006-01

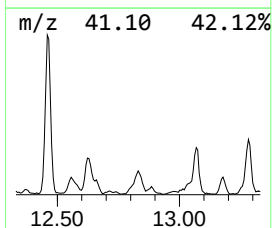
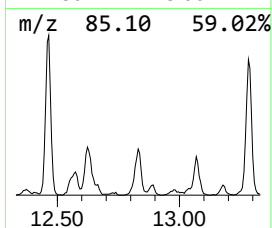
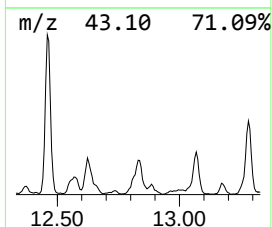
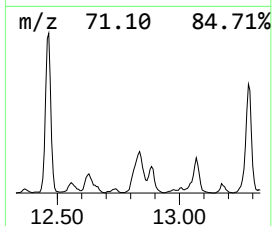
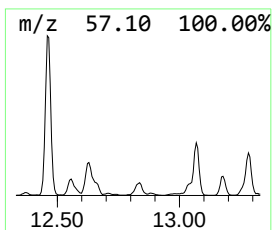
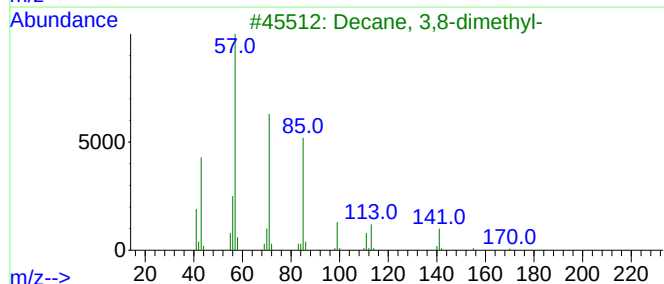
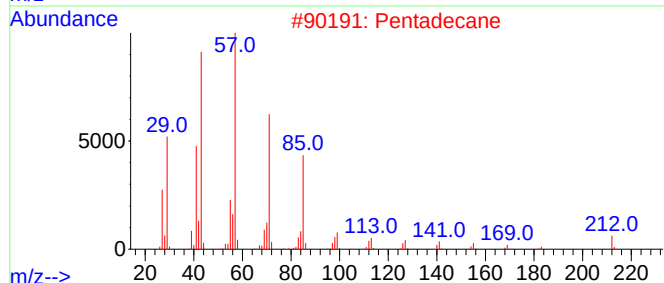
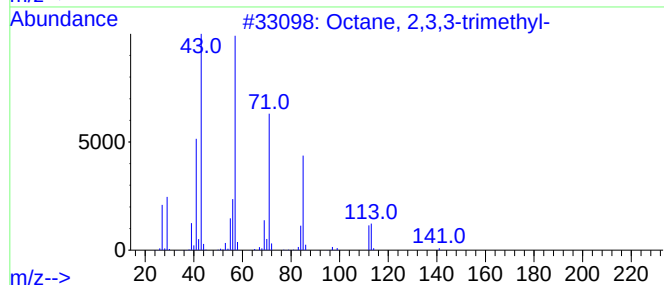
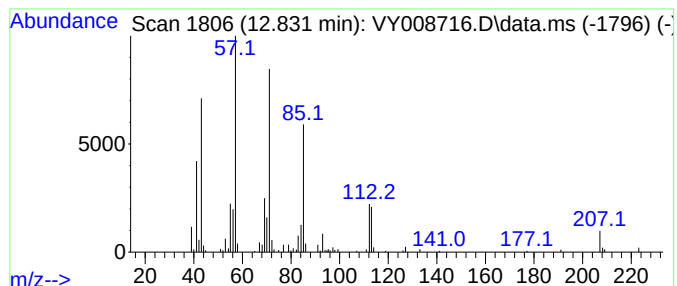
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050922S.M
Quant Title : SW846 8260

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

Peak Number 4 Octane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.831	11.70 ug/l	165483	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	78
2			Pentadecane	212	C15H32	000629-62-9	64
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	59
4			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	59
5			Nonadecane	268	C19H40	000629-92-5	59



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Misc : 5.33g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
P003-SS004-0006-01

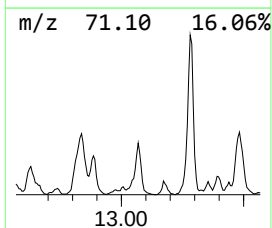
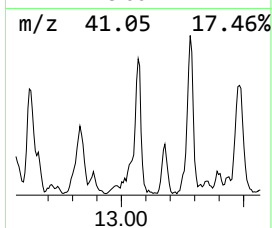
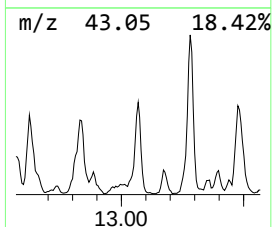
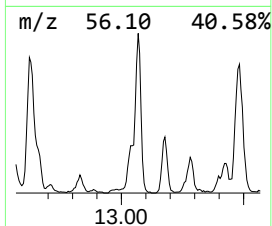
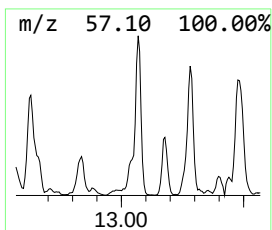
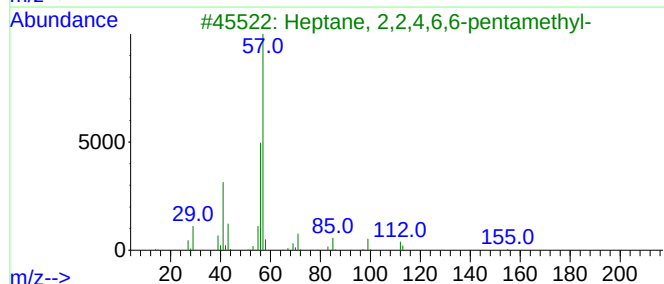
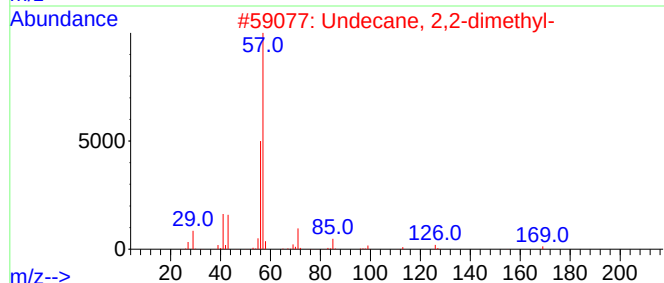
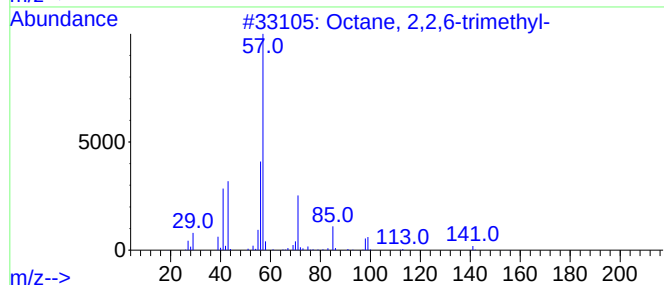
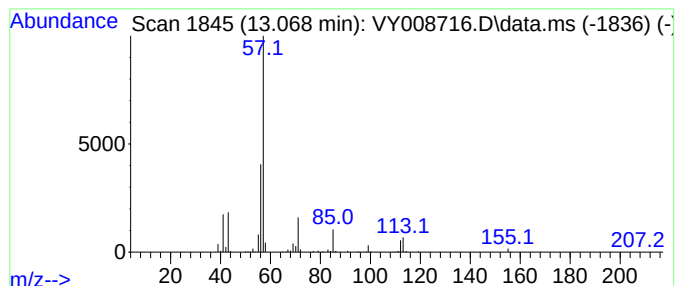
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050922S.M
Quant Title : SW846 8260

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

Peak Number 5 Octane, 2,2,6-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.068	17.23 ug/l	243683	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
2			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	72
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	64
5			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	64



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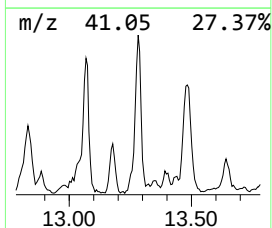
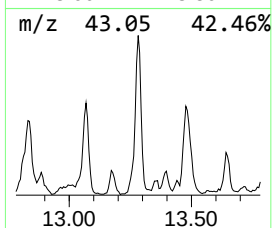
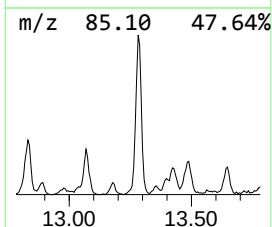
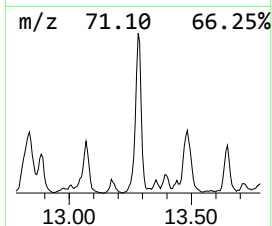
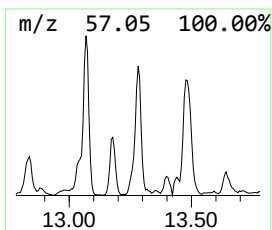
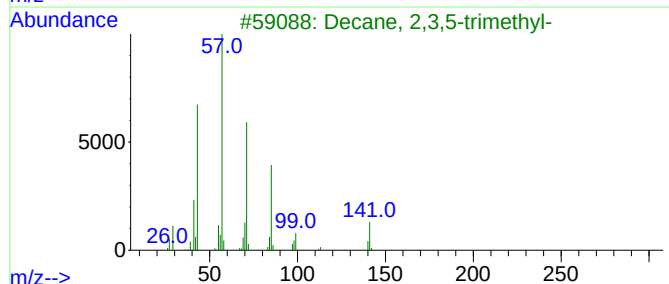
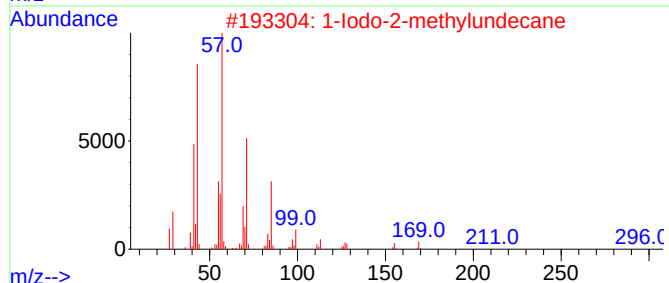
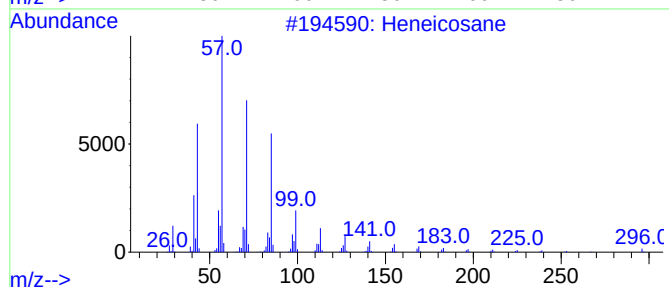
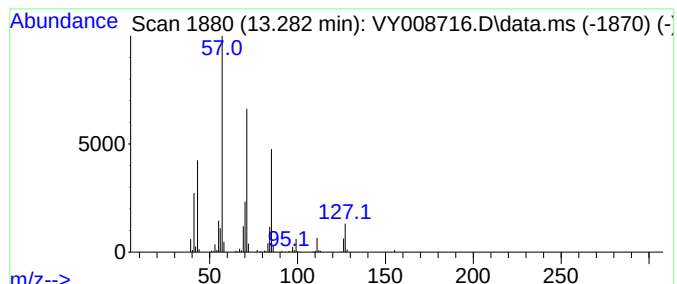
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050922S.M
Quant Title : SW846 8260

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

Peak Number 6 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	20.12 ug/l	284541	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	72
2			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	59
4			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
5			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051122\
Data File : VY008716.D
Acq On : 11 May 2022 18:47
Operator : KP/MD
Sample : N2781-06
Misc : 5.33g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
P003-SS004-0006-01

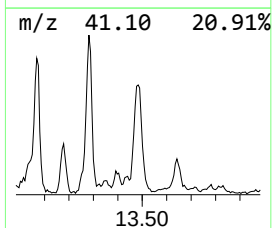
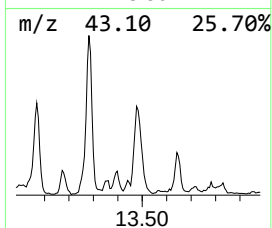
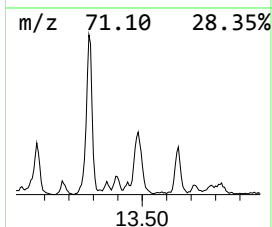
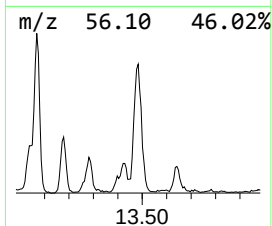
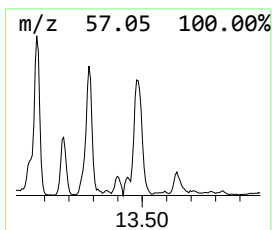
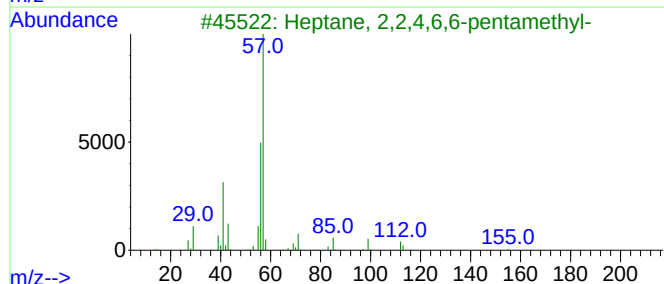
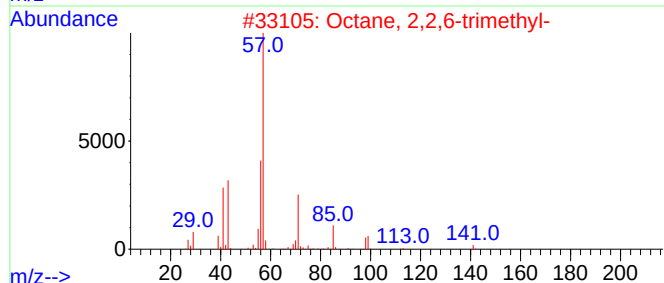
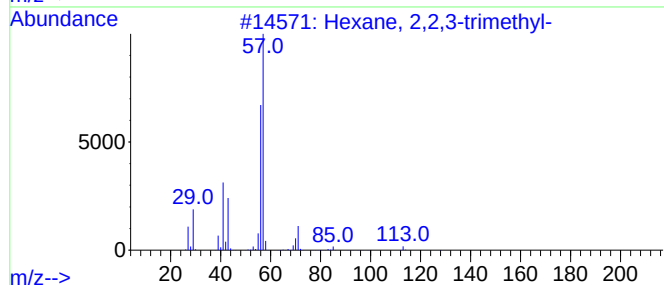
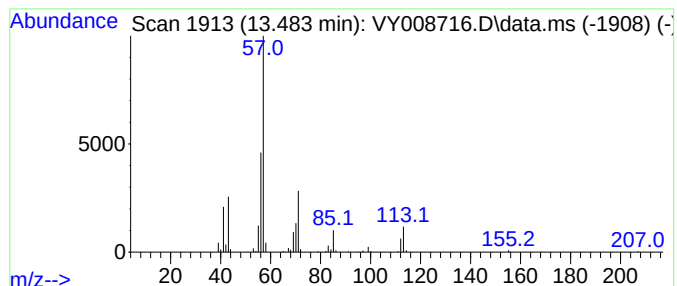
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.483	16.52 ug/l	233633	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	59
2			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	59
4			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	53
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051122\
Data File : VY008716.D
Acq On : 11 May 2022 18:47
Operator : KP/MD
Sample : N2781-06
Misc : 5.33g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
P003-SS004-0006-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050922S.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
2,2,7,7-Tetrame...	12.556	6.3	ug/l	89744	4	13.428	707136	50.0
Decane, 2,2-dim...	12.623	14.1	ug/l	199476	4	13.428	707136	50.0
Octane, 2,3,3-t...	12.831	11.7	ug/l	165483	4	13.428	707136	50.0
Octane, 2,2,6-t...	13.068	17.2	ug/l	243683	4	13.428	707136	50.0
Heneicosane	13.282	20.1	ug/l	284541	4	13.428	707136	50.0
Hexane, 2,2,3-t...	13.483	16.5	ug/l	233633	4	13.428	707136	50.0