

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
 Data File : VY006575.D
 Acq On : 02 Nov 2021 14:17
 Operator : SY/MD
 Sample : M4427-03
 Misc : 3.90G/5ML/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 FDR-BH-4-20211029-7.5-8

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\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.229	61	67	78	rVB	36196	63240	1.12%	0.111%
2	3.954	339	350	364	rBV2	50758	145472	2.57%	0.256%
3	6.990	838	848	863	rBV3	27853	91725	1.62%	0.161%
4	7.728	957	969	974	rBV	107226	258711	4.58%	0.455%
5	7.795	974	980	989	rVB	194048	436266	7.72%	0.768%
6	8.148	1029	1038	1049	rBV	131070	287738	5.09%	0.506%
7	8.557	1097	1105	1113	rBV	29113	62528	1.11%	0.110%
8	8.697	1120	1128	1135	rBV	314132	620565	10.98%	1.092%
9	8.776	1135	1141	1150	rVB	53261	101104	1.79%	0.178%
10	9.142	1194	1201	1213	rBV2	33698	78987	1.40%	0.139%
11	9.526	1257	1264	1273	rVB3	33329	82427	1.46%	0.145%
12	9.618	1273	1279	1285	rBV	32308	61526	1.09%	0.108%
13	9.752	1295	1301	1314	rVB2	40997	88467	1.57%	0.156%
14	10.117	1356	1361	1366	rVB	52081	77885	1.38%	0.137%
15	10.184	1366	1372	1381	rVB	502276	870906	15.41%	1.532%
16	10.691	1450	1455	1463	rVB	53129	101638	1.80%	0.179%
17	10.831	1475	1478	1485	rVB2	62875	107508	1.90%	0.189%
18	10.965	1496	1500	1505	rBV2	32089	70559	1.25%	0.124%
19	11.148	1526	1530	1536	rVV	45077	80703	1.43%	0.142%
20	11.221	1537	1542	1546	rVV2	50578	112153	1.99%	0.197%
21	11.264	1546	1549	1556	rVB2	79400	136740	2.42%	0.241%
22	11.495	1576	1587	1592	rBV	425825	748516	13.25%	1.317%
23	11.745	1623	1628	1633	rBV3	49654	94932	1.68%	0.167%
24	11.855	1642	1646	1648	rBV3	36084	59373	1.05%	0.104%
25	12.007	1664	1671	1674	rBV7	24449	66043	1.17%	0.116%
26	12.239	1706	1709	1713	rVV3	62539	98507	1.74%	0.173%
27	12.391	1725	1734	1739	rBV4	183568	481904	8.53%	0.848%
28	12.483	1744	1749	1754	rVV2	482143	932587	16.51%	1.641%
29	12.538	1754	1758	1768	rVB2	261095	742900	13.15%	1.307%
30	12.629	1768	1773	1776	rBV	116358	218082	3.86%	0.384%
31	12.708	1782	1786	1789	rBV2	125816	202356	3.58%	0.356%
32	12.788	1794	1799	1803	rBV2	243344	402587	7.13%	0.708%
33	12.830	1803	1806	1812	rVV4	74639	148213	2.62%	0.261%
34	12.891	1812	1816	1821	rVV3	106555	172886	3.06%	0.304%
35	13.074	1834	1846	1853	rBV3	2452858	5112694	90.49%	8.996%
36	13.141	1853	1857	1859	rVV2	221823	315438	5.58%	0.555%

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37	13.178	1859	1863	1870	rVB3	496562	924547	16.36%	1.627%
38	13.257	1871	1876	1877	rBV2	162291	255407	4.52%	0.449%
39	13.288	1877	1881	1885	rVV3	301145	539143	9.54%	0.949%
40	13.355	1887	1892	1897	rVV	1501499	2570083	45.49%	4.522%
41	13.416	1897	1902	1909	rVB2	1216972	2470239	43.72%	4.347%
42	13.513	1909	1918	1922	rBV5	636471	1507241	26.68%	2.652%
43	13.617	1929	1935	1941	rBV5	948893	2341378	41.44%	4.120%
44	13.678	1941	1945	1948	rVV	585005	877146	15.52%	1.543%
45	13.714	1948	1951	1957	rVB3	592327	1178314	20.86%	2.073%
46	13.788	1957	1963	1970	rBV2	3187134	5649922	100.00%	9.941%
47	13.855	1970	1974	1980	rVV2	1276298	1989696	35.22%	3.501%
48	13.952	1986	1990	1995	rBV4	276268	612978	10.85%	1.079%
49	14.007	1996	1999	2002	rVV2	375759	558682	9.89%	0.983%
50	14.044	2002	2005	2007	rVV3	548764	843151	14.92%	1.484%
51	14.080	2007	2011	2016	rVV	3449978	5383055	95.28%	9.472%
52	14.135	2017	2020	2025	rVB3	707720	1124971	19.91%	1.979%
53	14.269	2037	2042	2043	rBV2	319049	478447	8.47%	0.842%
54	14.379	2052	2060	2063	rBV4	647062	1220452	21.60%	2.147%
55	14.531	2082	2085	2089	rBV	437106	653477	11.57%	1.150%
56	14.617	2095	2099	2104	rVB3	372891	642039	11.36%	1.130%
57	14.720	2111	2116	2118	rBV3	343557	614758	10.88%	1.082%
58	14.757	2118	2122	2132	rVB	1332004	2392089	42.34%	4.209%
59	14.854	2133	2138	2141	rBV3	362727	722889	12.79%	1.272%
60	14.952	2148	2154	2162	rVB8	419667	1201553	21.27%	2.114%
61	15.062	2169	2172	2175	rBV2	176249	195390	3.46%	0.344%
62	15.220	2194	2198	2201	rVB	308279	457211	8.09%	0.804%
63	15.281	2205	2208	2214	rVB3	349112	627349	11.10%	1.104%
64	15.342	2215	2218	2223	rVB2	228979	354637	6.28%	0.624%
65	15.501	2239	2244	2251	rBV2	1245922	2524683	44.69%	4.442%
66	15.568	2252	2255	2259	rVV4	397257	656209	11.61%	1.155%
67	15.879	2302	2306	2314	rBV4	250315	605601	10.72%	1.066%
68	16.007	2323	2327	2338	rVB5	270976	925225	16.38%	1.628%

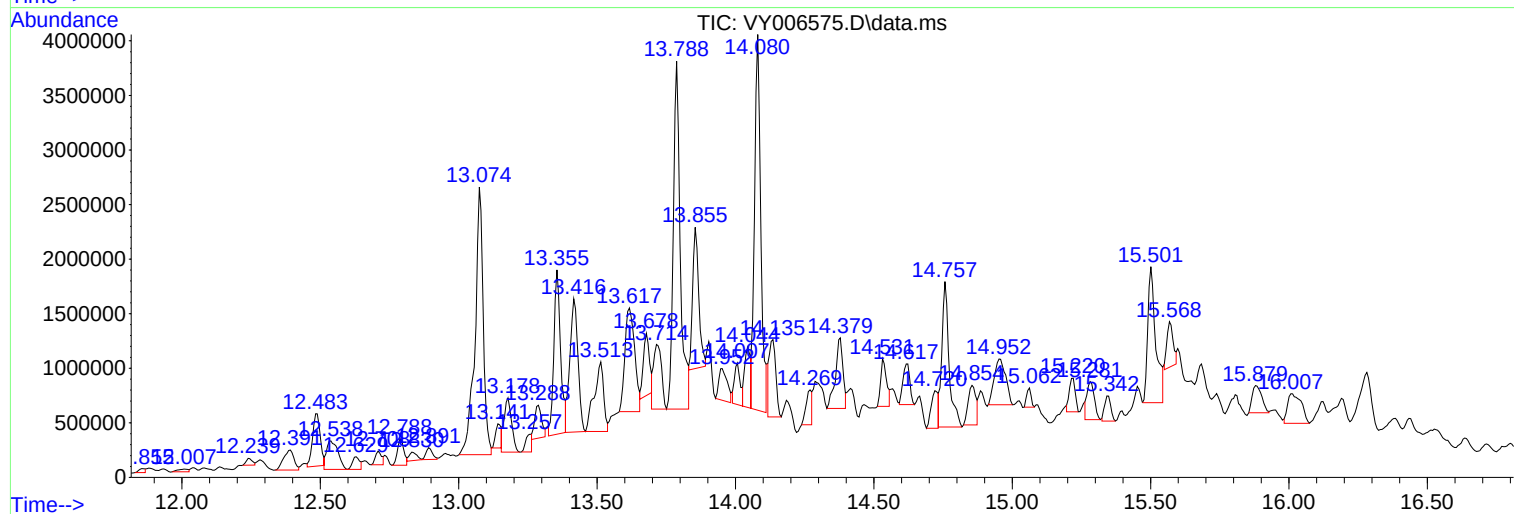
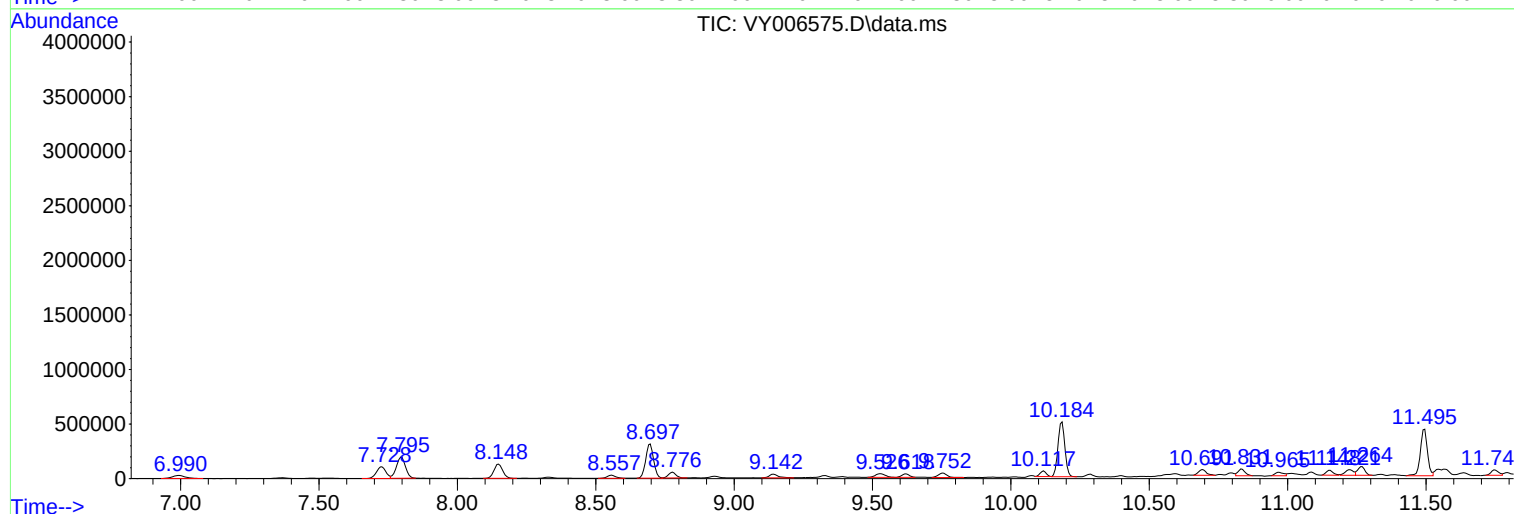
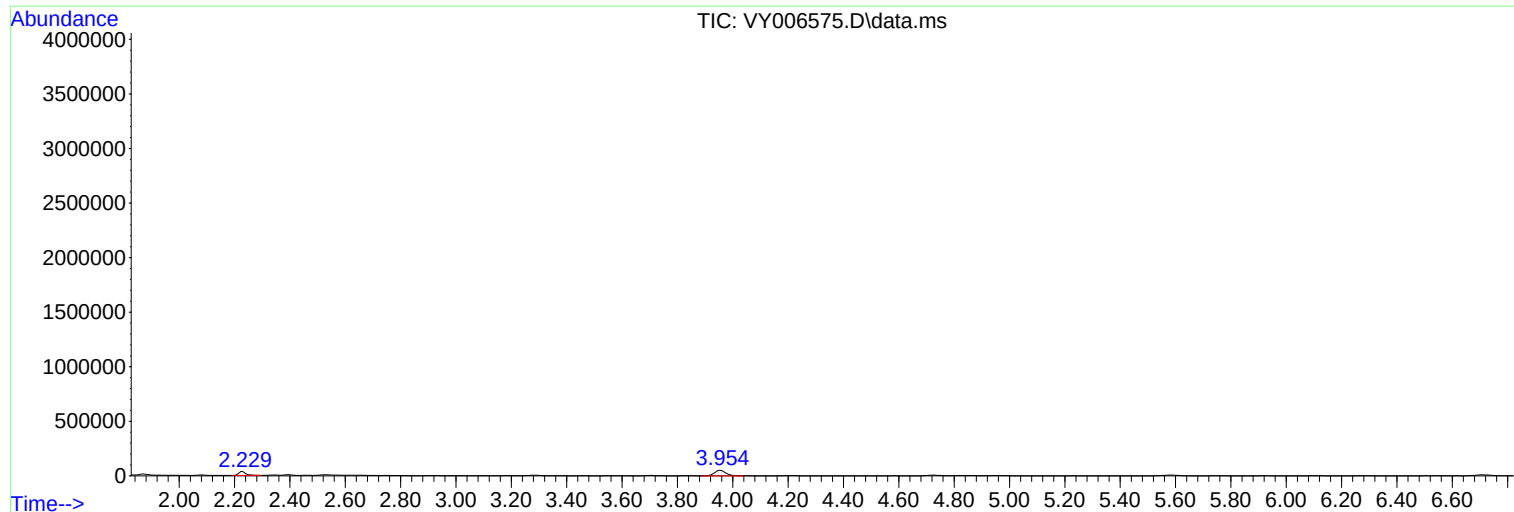
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

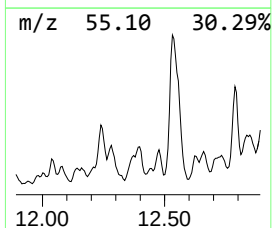
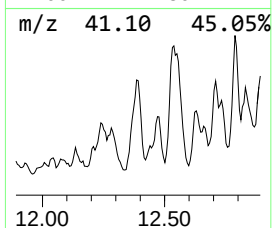
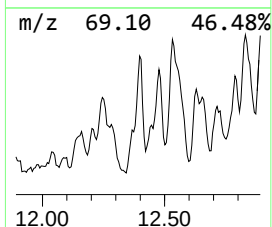
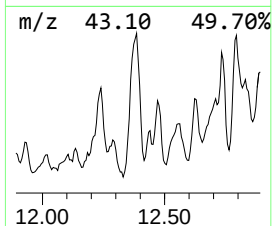
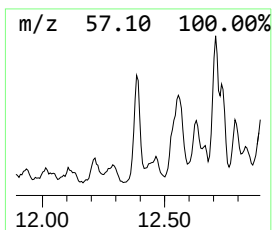
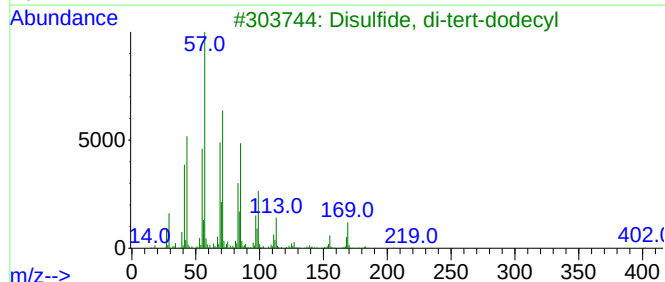
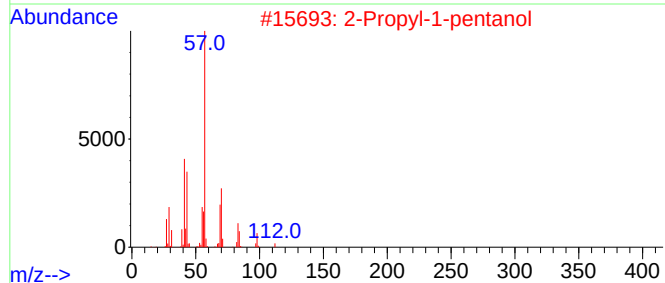
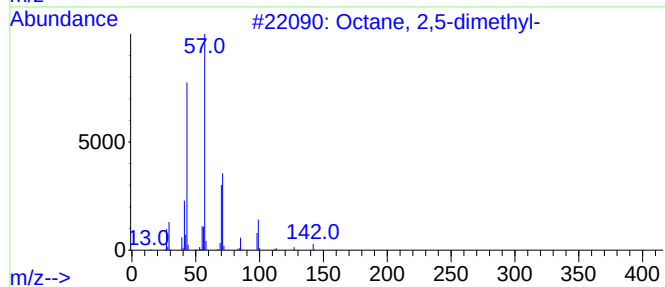
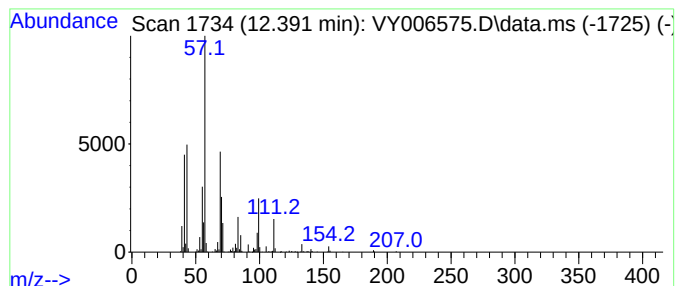
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown12.391 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.391	32.19 ug/l	481904	Chlorobenzene-d5	11.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	43
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43
3			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	42
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	40
5			4,4-Dimethyl octane	142	C10H22	015869-95-1	37



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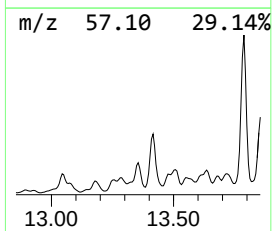
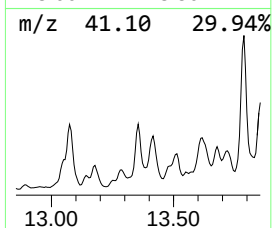
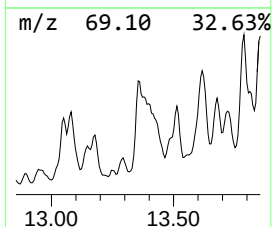
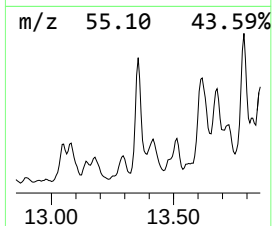
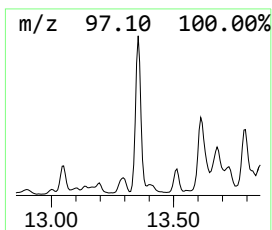
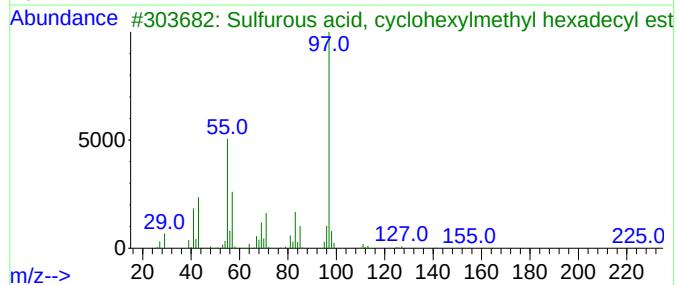
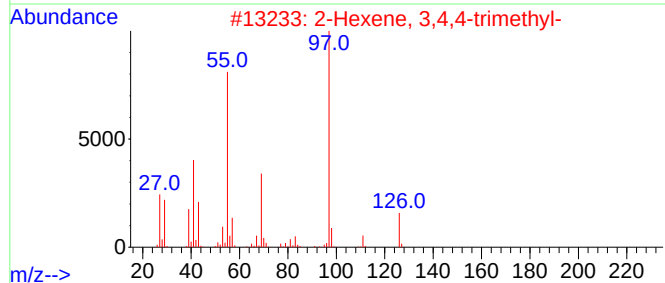
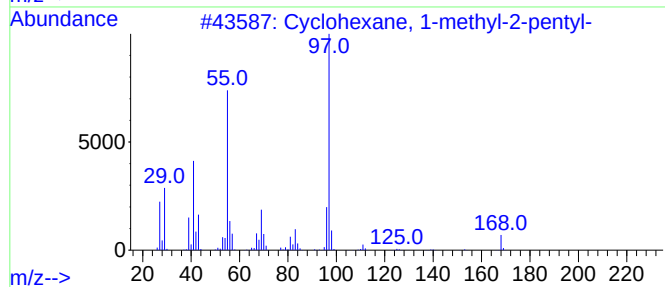
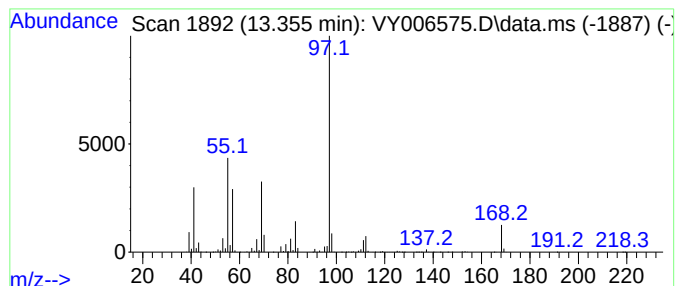
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, 1-methyl-2-pen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.355	52.02 ug/l	2570080	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	78
2			2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	64
3			Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	64
4			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	64
5			Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	64



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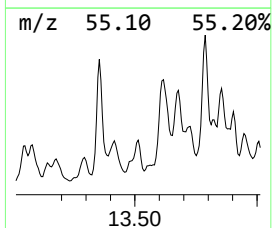
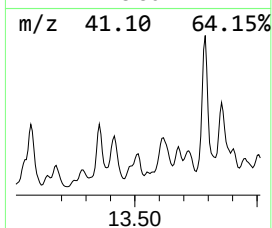
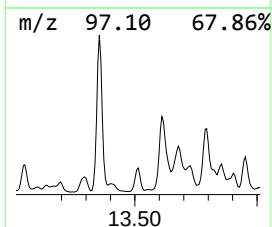
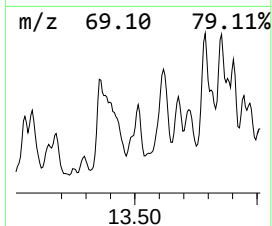
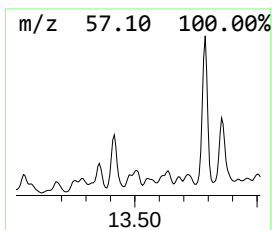
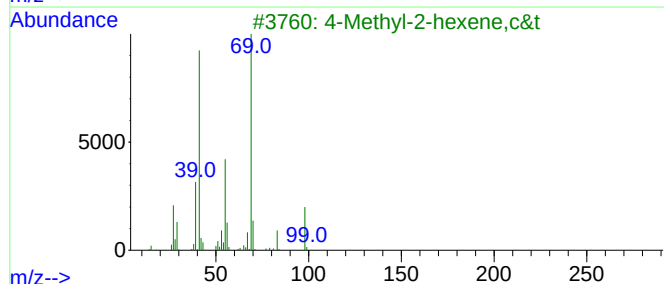
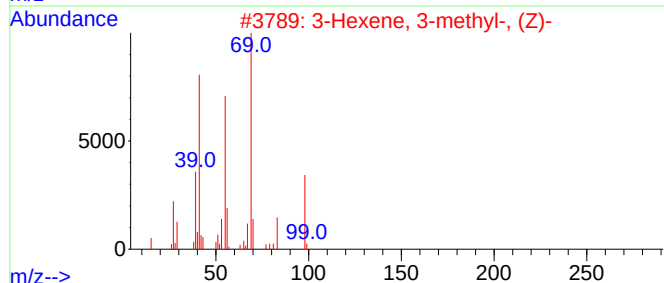
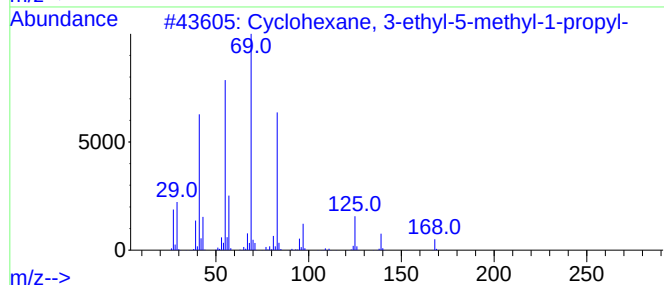
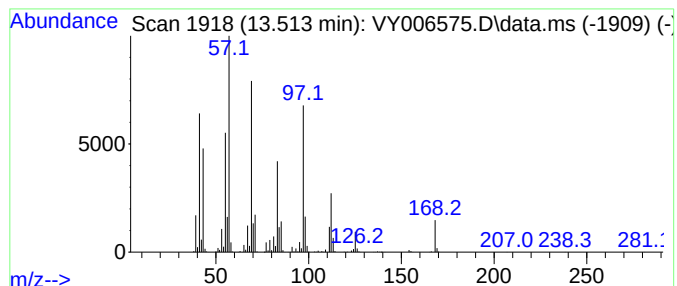
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown13.513 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	30.51 ug/l	1507240	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 3-ethyl-5-methyl-1-...	168	C12H24	1000151-39-5	43
2			3-Hexene, 3-methyl-, (Z)-	98	C7H14	004914-89-0	42
3			4-Methyl-2-hexene,c&t	98	C7H14	003404-55-5	38
4			3-Hexene, 2-methyl-, (Z)-	98	C7H14	015840-60-5	38
5			Formaldehyde, (2-butenyl)methylh...	112	C6H12N2	068661-51-8	38



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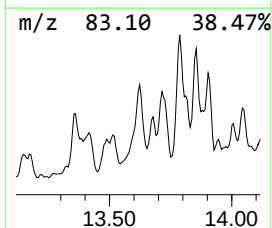
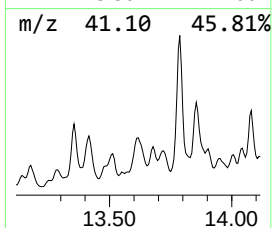
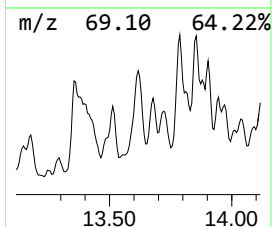
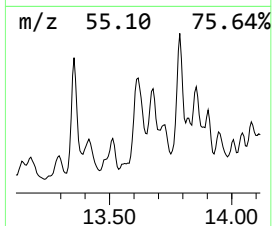
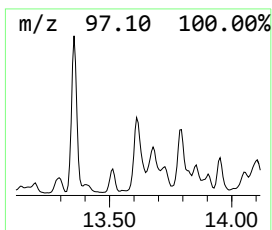
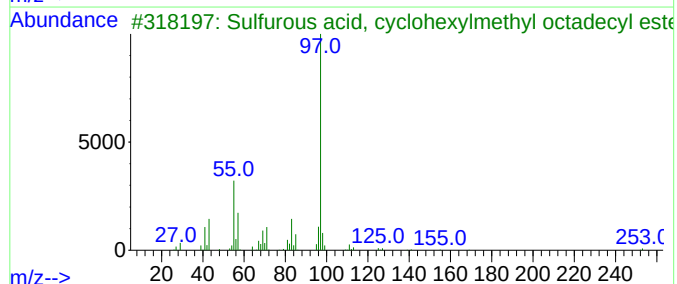
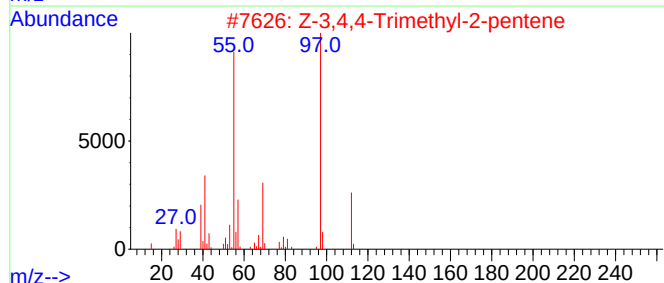
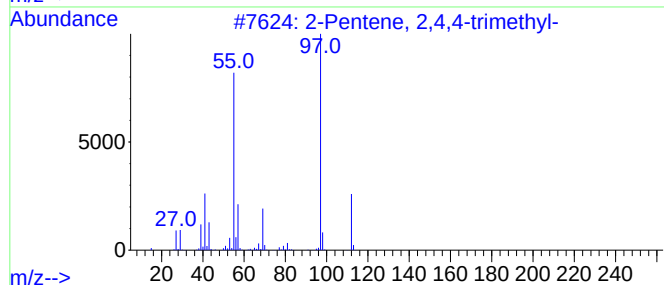
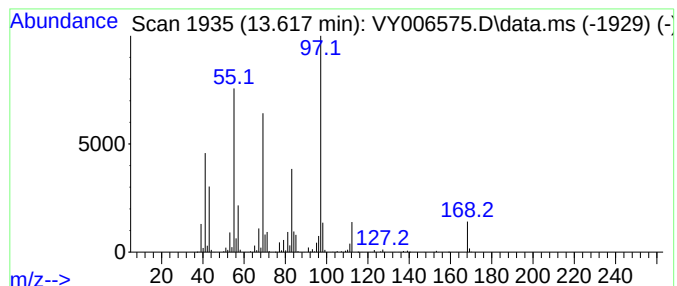
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.617 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.617	47.39 ug/l	2341380	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	49
2			Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	49
3			Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	47
4			Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	47
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

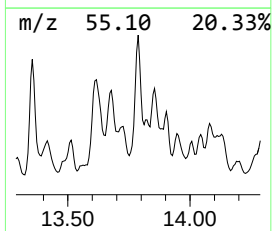
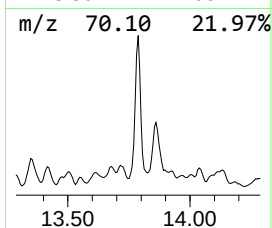
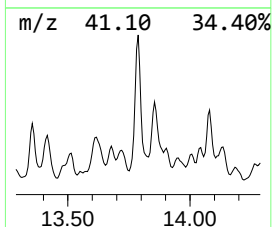
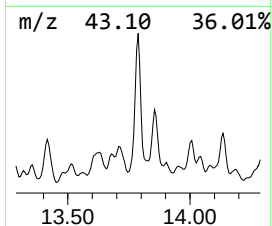
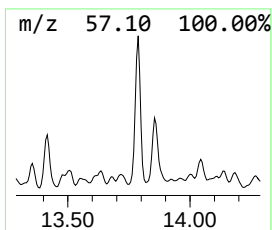
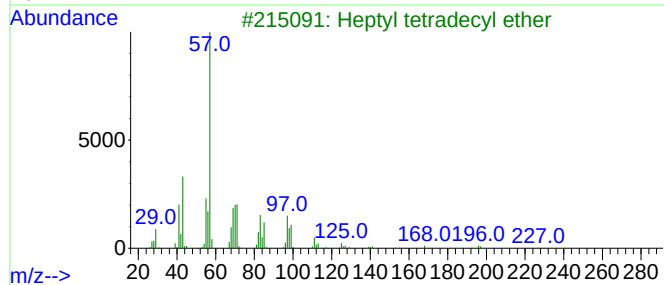
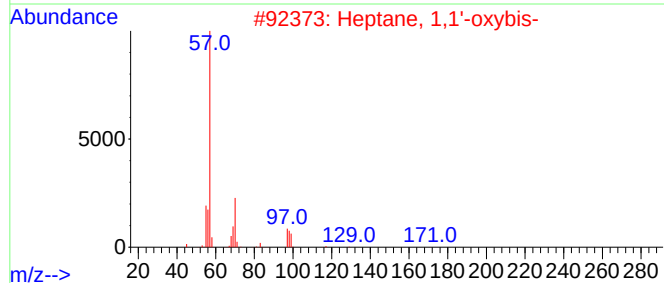
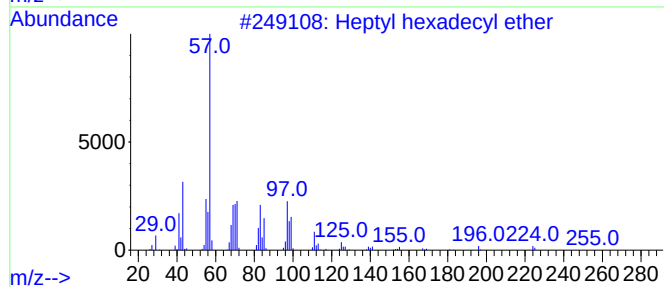
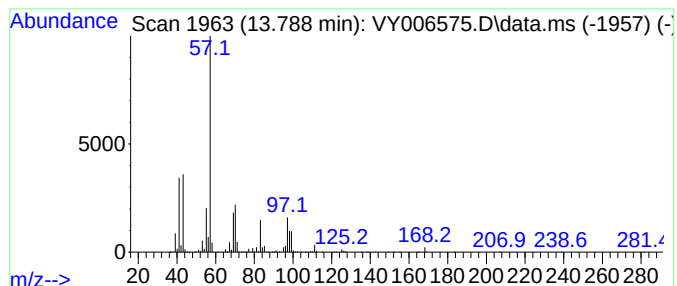
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Quant Title : SW846 8260

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

Peak Number 5 Heptyl hexadecyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	114.36 ug/l	5649920	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl hexadecyl ether	340	C23H48O	1000406-39-4	72
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	56
3			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	56
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

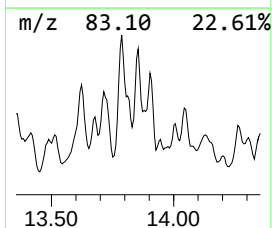
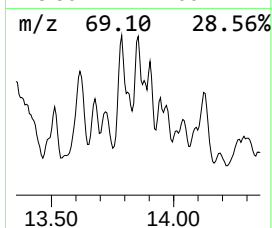
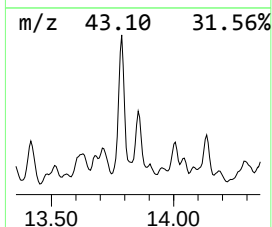
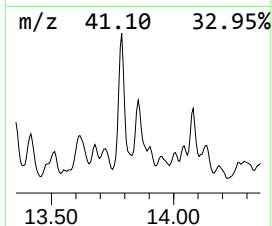
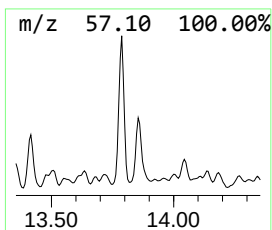
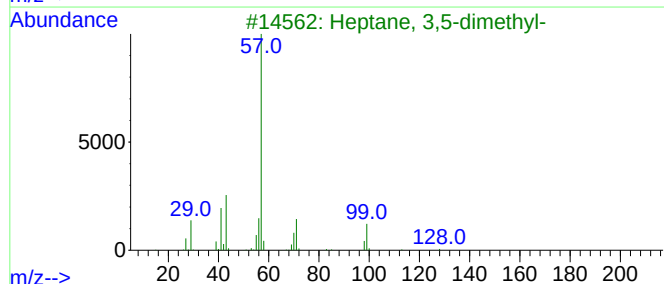
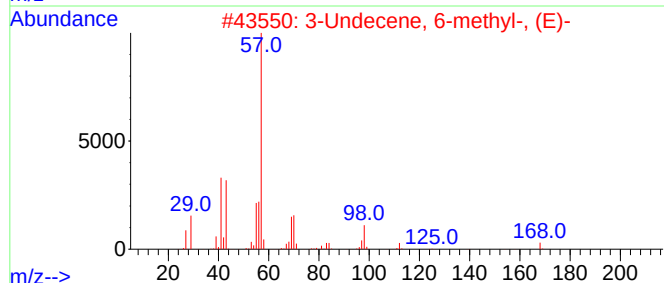
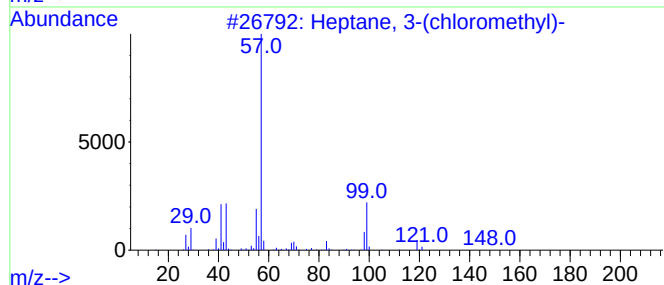
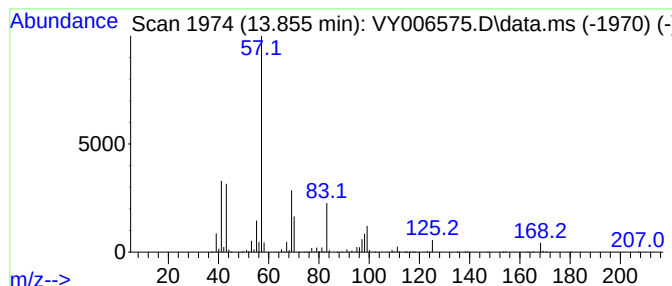
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.855 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.855	40.27 ug/l	1989700	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-(chloromethyl)-	148	C8H17Cl	000123-04-6	38
2			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	38
3			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38
4			2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	38
5			2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

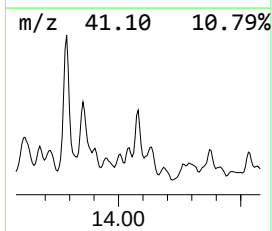
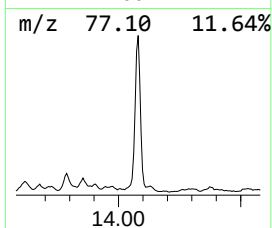
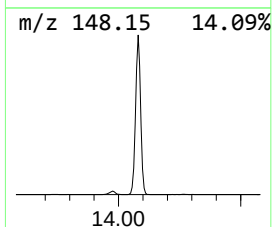
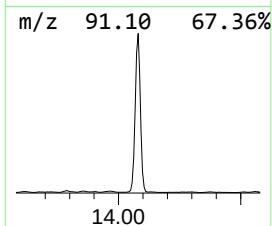
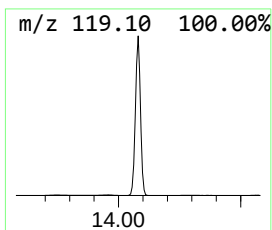
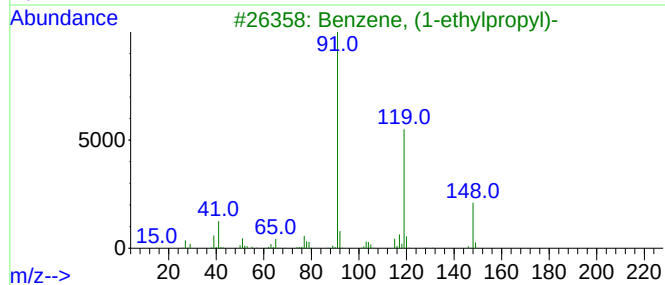
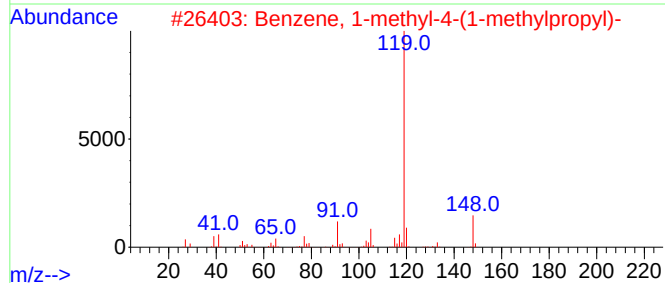
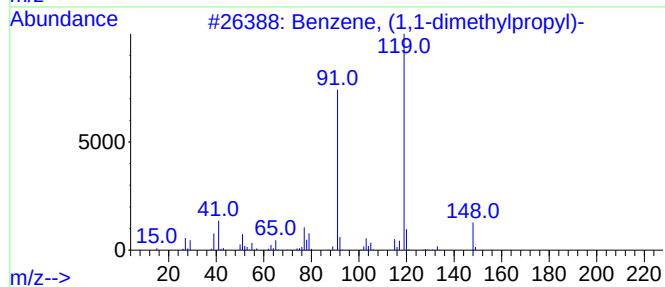
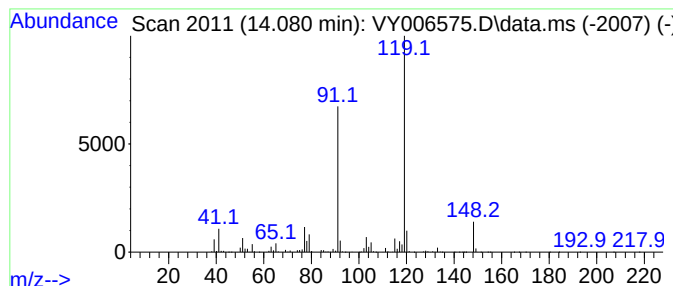
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1,1-dimethylpropyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	108.96 ug/l	5383060	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	97
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	90
3			Benzene, (1-ethylpropyl)-	148	C11H16	001196-58-3	86
4			Benzene, tert-butyl-	134	C10H14	000098-06-6	86
5			Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

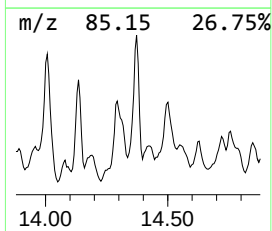
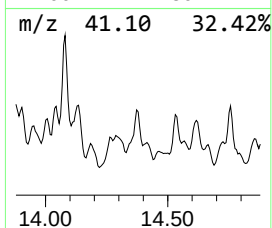
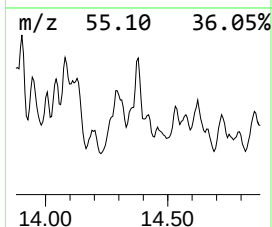
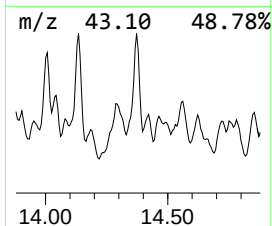
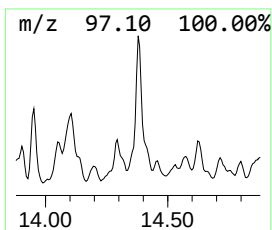
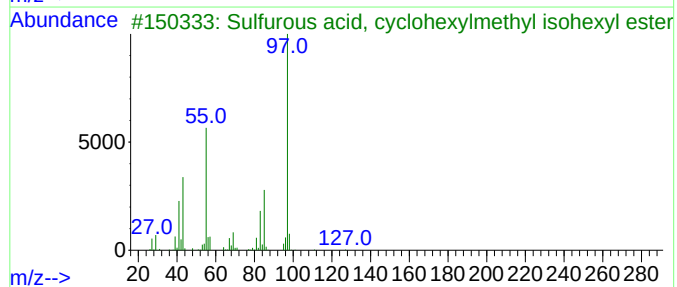
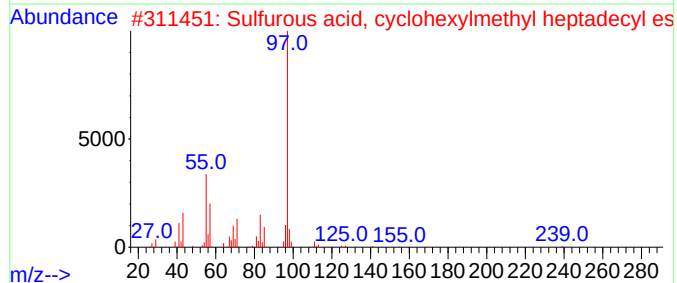
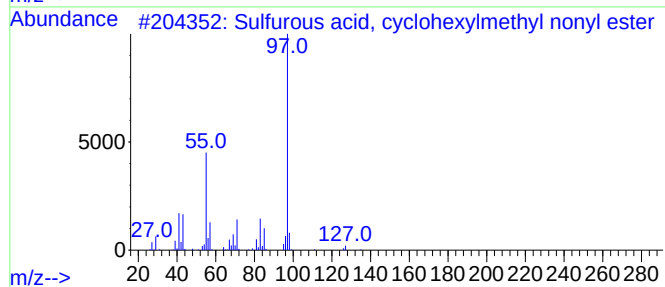
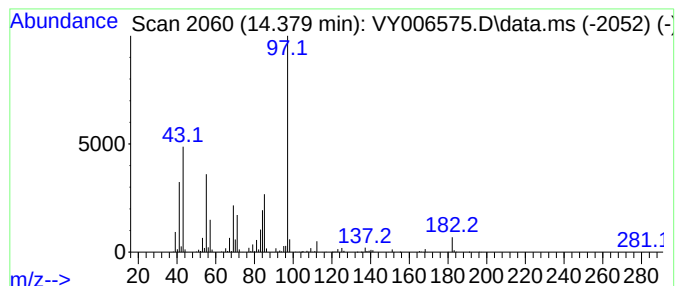
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Quant Title : SW846 8260

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

Peak Number 8 Sulfurous acid, cyclohexylm... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.379	24.70 ug/l	1220450	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	53
2			Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	53
3			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	50
4			Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	42
5			Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

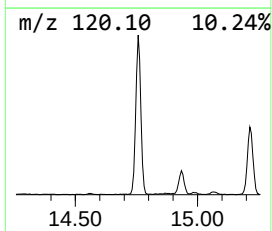
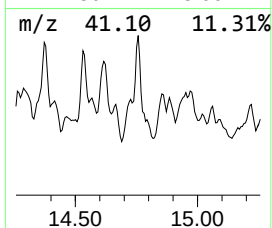
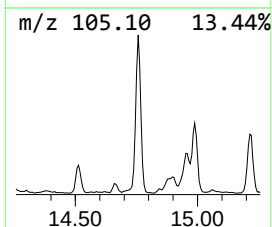
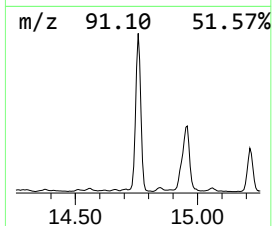
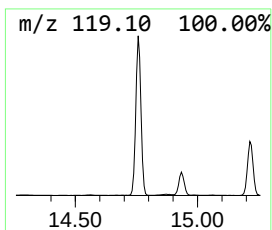
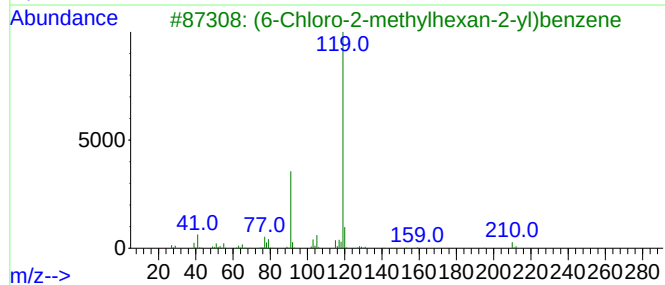
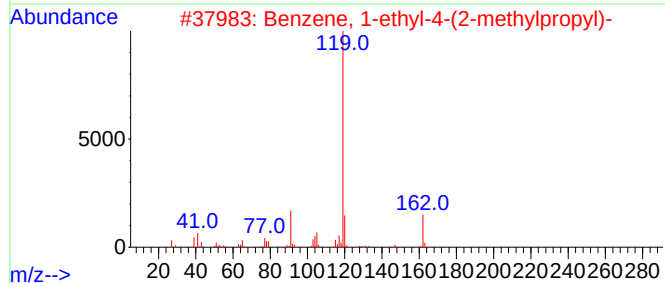
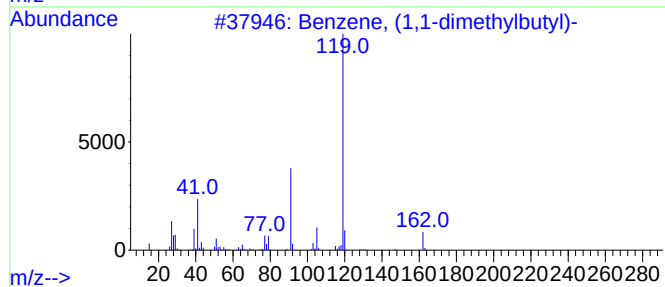
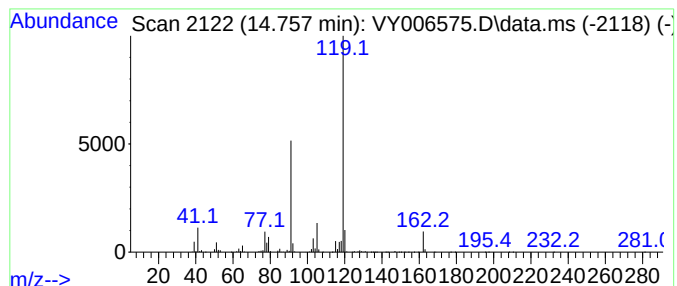
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1,1-dimethylbutyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	48.42 ug/l	2392090	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	91
2			Benzene, 1-ethyl-4-(2-methylprop...	162	C12H18	100319-40-2	91
3			(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	86
4			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78
5			Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

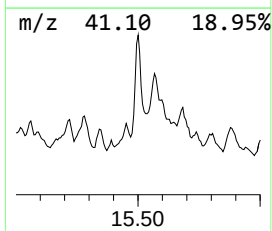
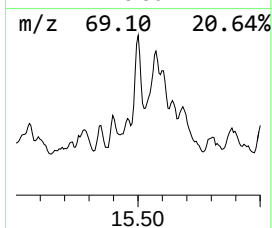
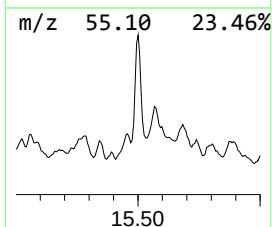
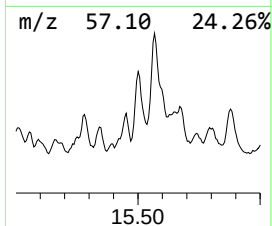
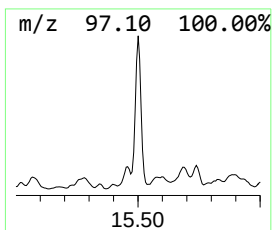
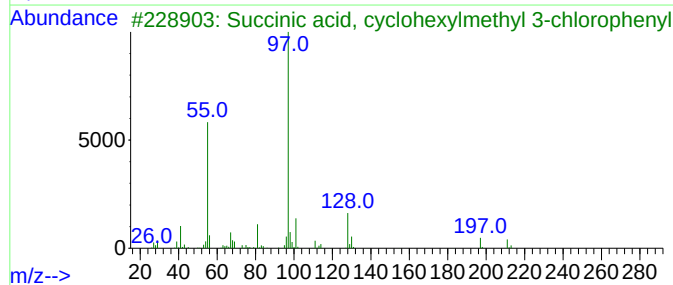
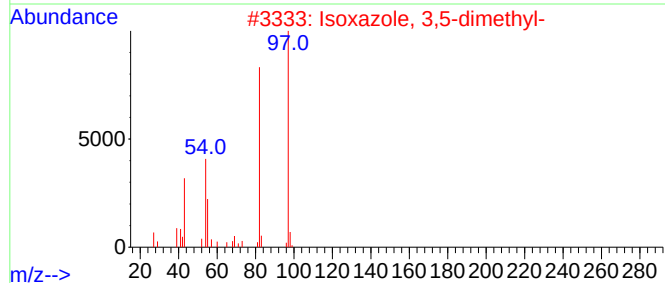
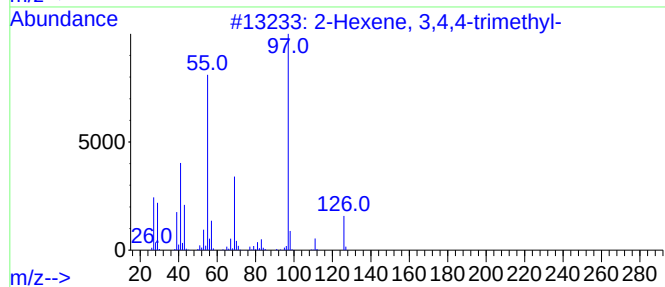
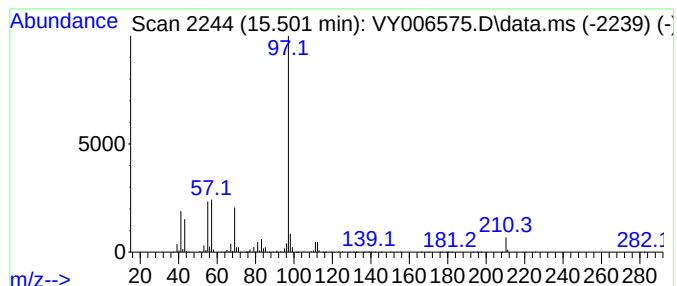
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 10 2-Hexene, 3,4,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	51.10 ug/l	2524680	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	64		
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	59		
3	Succinic acid, cyclohexylmethyl ...	324	C17H21ClO4	1010389-85-4	56		
4	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	56		
5	Succinic acid, cyclohexylmethyl ...	392	C17H19Cl3O4	1000389-96-9	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006575.D
Acq On : 02 Nov 2021 14:17
Operator : SY/MD
Sample : M4427-03
Misc : 3.90G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.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
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Cyclohexane, 1-...	13.355	52.0	ug/l	2570080	4	13.428	2470240	50.0
unknown13.513	13.513	30.5	ug/l	1507240	4	13.428	2470240	50.0
unknown13.617	13.617	47.4	ug/l	2341380	4	13.428	2470240	50.0
Heptyl hexadecy...	13.788	114.4	ug/l	5649920	4	13.428	2470240	50.0
unknown13.855	13.855	40.3	ug/l	1989700	4	13.428	2470240	50.0
Benzene, (1,1-d...	14.080	109.0	ug/l	5383060	4	13.428	2470240	50.0
Sulfurous acid,...	14.379	24.7	ug/l	1220450	4	13.428	2470240	50.0
Benzene, (1,1-d...	14.757	48.4	ug/l	2392090	4	13.428	2470240	50.0
2-Hexene, 3,4,4...	15.501	51.1	ug/l	2524680	4	13.428	2470240	50.0