LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

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: VY006587.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	77	rVB	49913	86431	1.05%	0.129%
2	3.954	339	350	366	rBV2	64185	180961	2.19%	0.270%
3	6.990	837	848	863	rBV2	36461	119852	1.45%	0.179%
4	7.728	957	969	974	rBV	97865	232689	2.82%	0.347%
5	7.795	974	980	989	rVB	177696	392430	4.76%	0.585%
6	8.149	1028	1038	1047	rBV	117815	262839	3.19%	0.392%
7	8.697	1120	1128	1135	rBV	281853	552595	6.70%	0.823%
8	8.776	1135	1141	1150	rVB	52806	102653	1.24%	0.153%
9	9.142	1193	1201	1214	rVB	45561	98144	1.19%	0.146%
10	9.526	1255	1264	1273	rVB3	45910	115350	1.40%	0.172%
11	9.752	1293	1301	1310	rBV2	58113	119800	1.45%	0.179%
12	10.118	1356	1361	1366	rVB2	85413	140024	1.70%	0.209%
13	10.185	1366	1372	1383	rVB	459465	798560	9.68%	1.190%
14	10.691	1448	1455	1462	rBV2	70987	143426	1.74%	0.214%
15	10.831	1474	1478	1486	rVB2	104538	193298	2.34%	0.288%
16	10.965	1494	1500	1506	rBV3	58926	139824	1.70%	0.208%
17	11.087	1515	1520	1526	rVB	56351	97012	1.18%	0.145%
18	11.148	1526	1530	1536	rVV	65908	114948	1.39%	0.171%
19	11.227	1536	1543	1546	rVV2	68730	163310	1.98%	0.243%
20	11.264	1546	1549	1557	rVB2	140366	245498	2.98%	0.366%
21	11.489	1576	1586	1592	rBV	394584	723899	8.78%	1.079%
22	11.544	1592	1595	1597	rBV2	61891	90782	1.10%	0.135%
23	11.745	1621	1628	1633	rBV2	79765	159728	1.94%	0.238%
24	11.855	1641	1646	1648	rBV3	65048	110304	1.34%	0.164%
25	11.886	1648	1651	1656	rVV3	73629	148087	1.80%	0.221%
26	12.142	1689	1693	1695	rBV4	57816	87794	1.06%	0.131%
27	12.245	1700	1710	1713	rBV4	165961	402613	4.88%	0.600%
28	12.282	1713	1716	1725	rVB4	162707	360418	4.37%	0.537%
29	12.392	1725	1734	1739	rBV4	333718	871075	10.56%	1.298%
30	12.483	1744	1749	1754	rBV3	461685	870194	10.55%	1.297%
31	12.538	1754	1758	1768	rVB3	456675	1278073	15.49%	1.904%
32	12.629	1768	1773	1776	rBV	192291	352368	4.27%	0.525%
33	12.709	1782	1786	1789	rBV	208271	333258	4.04%	0.497%
34	12.788	1794	1799	1803	rBV	406126	677645	8.22%	1.010%
35	12.831	1803	1806	1812	rVV3	120862	252735	3.06%	0.377%
36	12.892	1812	1816	1822	rVV5	164571	288194	3.49%	0.429%

LSC Area Percent Report

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Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

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

37	13.074	1834	1846	1854	rBV2	3951267	8248649	100.00%	12.292%
38	13.142	1854	1857	1859	rVV2	416300	616507	7.47%	0.919%
39	13.178	1859	1863	1870	rVB3	774171	1429721	17.33%	2.130%
40	13.288	1877	1881	1885	rBV3	398306	603944	7.32%	0.900%
41	13.355	1887	1892	1897	rVV2	2133555	3524178	42.72%	5.251%
42	13.416	1897	1902	1909	rVB	1522268	3062235	37.12%	4.563%
43	13.513	1909	1918	1922	rBV5	792279	1901343	23.05%	2.833%
44	13.611	1929	1934	1941	rBV5	1183872	2933616	35.56%	4.371%
45	13.678	1941	1945	1948	rVV	697307	1030281	12.49%	1.535%
46	13.721	1949	1952	1957	rVB2	735528	1313039	15.92%	1.957%
47	13.788	1957	1963	1970	rBV2	3997906	6841754	82.94%	10.195%
48	13.855	1970	1974	1980	rBV2	1485684	2328989	28.23%	3.471%
49	13.952	1986	1990	1995	rBV4	347790	654453	7.93%	0.975%
50	14.007	1996	1999	2001	rBV2	311271	336970	4.09%	0.502%
51	14.044	2002	2005	2006	rBV2	398123	438161	5.31%	0.653%
52	14.080	2006	2011	2016	rVB	4126407	5932402	71.92%	8.840%
53	14.184	2025	2028	2034	rVB4	311445	613516	7.44%	0.914%
54	14.269	2037	2042	2043	rBV2	330320	494575	6.00%	0.737%
55	14.379	2053	2060	2064	rBV3	646121	1177467	14.27%	1.755%
56	14.464	2071	2074	2076	rBV2	123373	192902	2.34%	0.287%
57	14.532	2082	2085	2089	rBV	404136	635652	7.71%	0.947%
58	14.617	2095	2099	2104	rVB3	393155	671886	8.15%	1.001%
59	14.721	2111	2116	2118	rBV2	333045	595664	7.22%	0.888%
60	14.757	2118	2122	2133	rVB	1413771	2418162	29.32%	3.603%
61	14.855	2133	2138	2141	rBV3	349327	679027	8.23%	1.012%
62	14.952	2148	2154	2162	rVB7	447501	1230273	14.91%	1.833%
63	15.062	2169	2172	2175	rBV2	165041	190769	2.31%	0.284%
64	15.220	2194	2198	2202	rVB	302306	452784	5.49%	0.675%
65	15.281	2205	2208	2214	rVB2	325116	596256	7.23%	0.888%
66	15.342	2215	2218	2223	rVB3	221748	330751	4.01%	0.493%
67	15.501	2239	2244	2251	rBV2	1243343	2465399	29.89%	3.674%
68	15.568	2252	2255	2259	rVV2	377390	618699	7.50%	0.922%
69	15.879	2302	2306	2314	rVB2	309535	762080	9.24%	1.136%
70	16.013	2323	2328	2330	rBV3	254645	479253	5.81%	0.714%

Sum of corrected areas: 67108168

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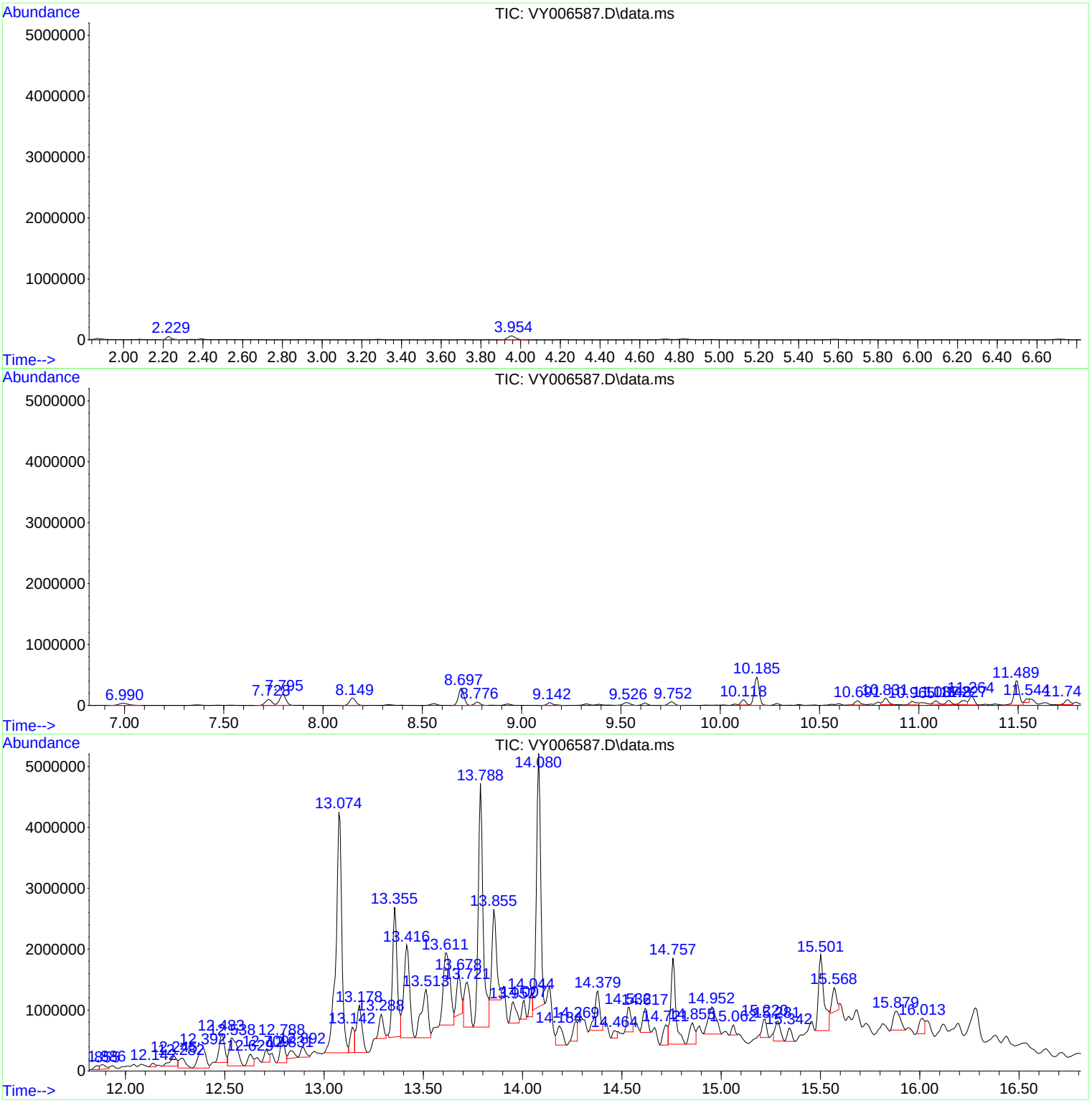
Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8M

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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Sample : M4427-04
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FDR-BH-4-20211029-7.5-8M

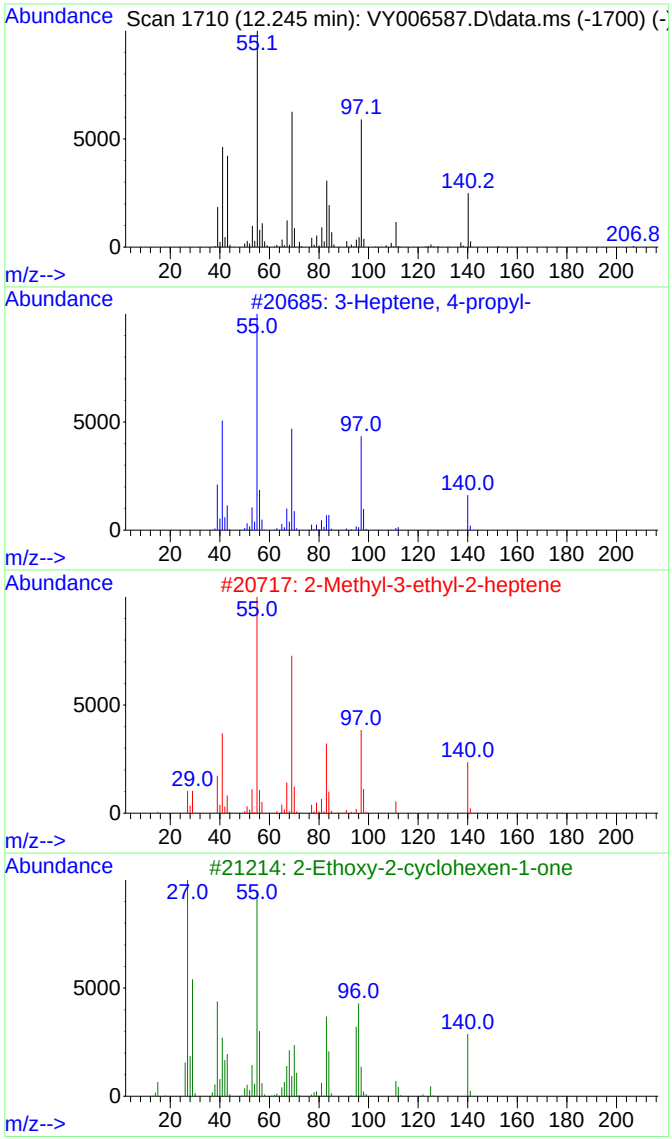
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

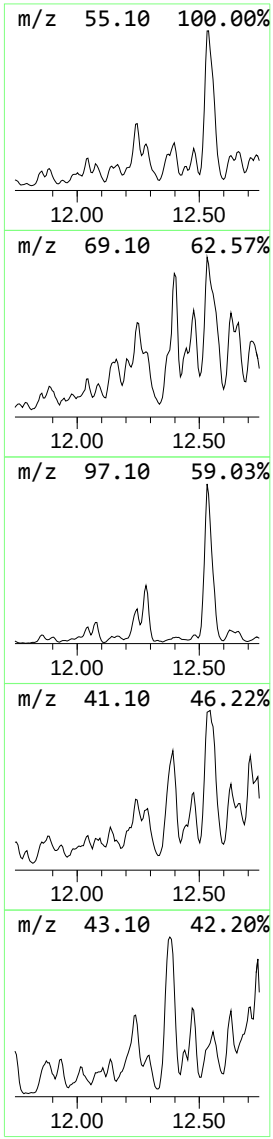
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Heptene, 4-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.245	27.81 ug/l	402613	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	64
2	2-Methyl-3-ethyl-2-heptene	140	C10H20	019780-61-1	53
3	2-Ethoxy-2-cyclohexen-1-one	140	C8H12O2	029941-82-0	50
4	Semustine	247	C10H18ClN3O2	013909-09-6	47
5	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

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

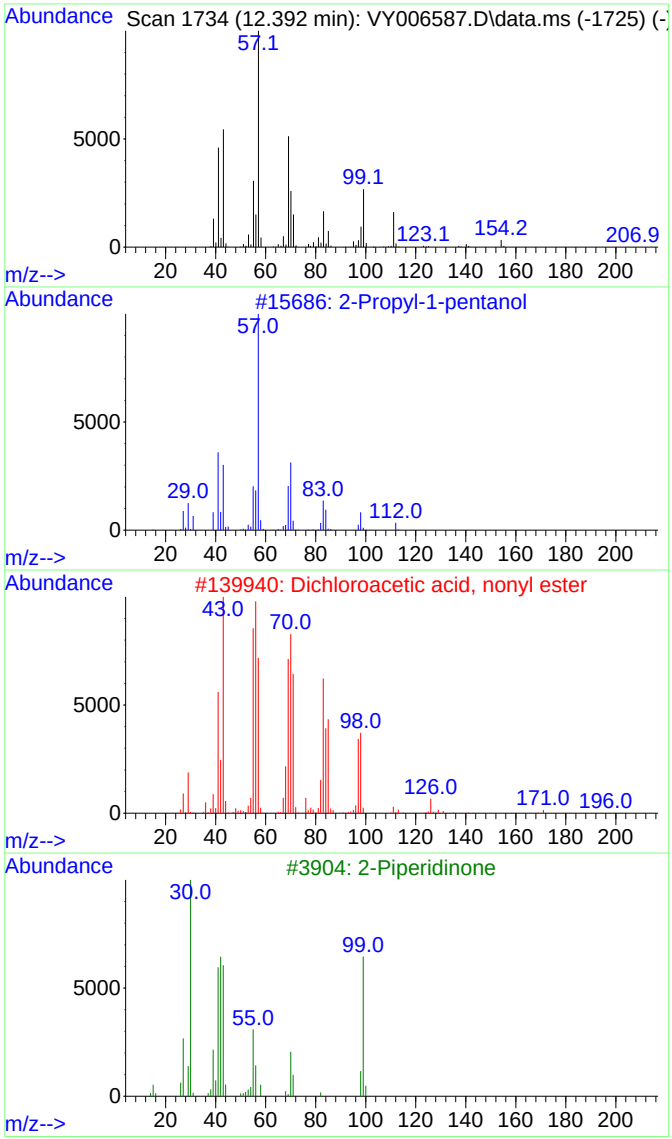
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

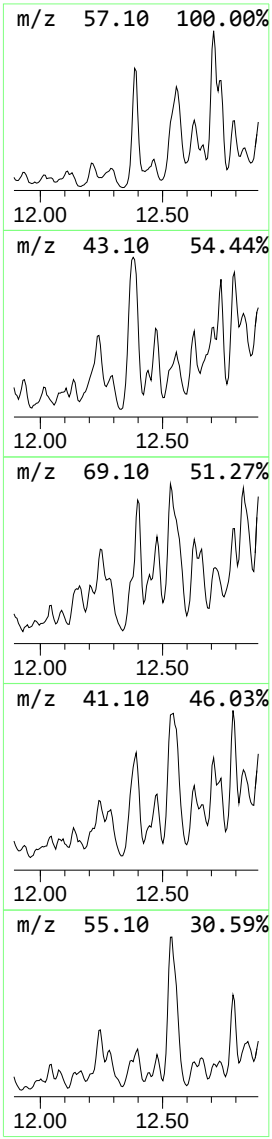
****

Peak Number 2 2-Propyl-1-pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	60.17 ug/l	871075	Chlorobenzene-d5	11.496

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
2	Dichloroacetic acid, nonyl ester	254	C11H20Cl2O2	083004-99-3	47
3	2-Piperidinone	99	C5H9NO	000675-20-7	43
4	Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	43
5	Oxirane, (1,1-dimethylbutyl)-	128	C8H16O	053907-76-9	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
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Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

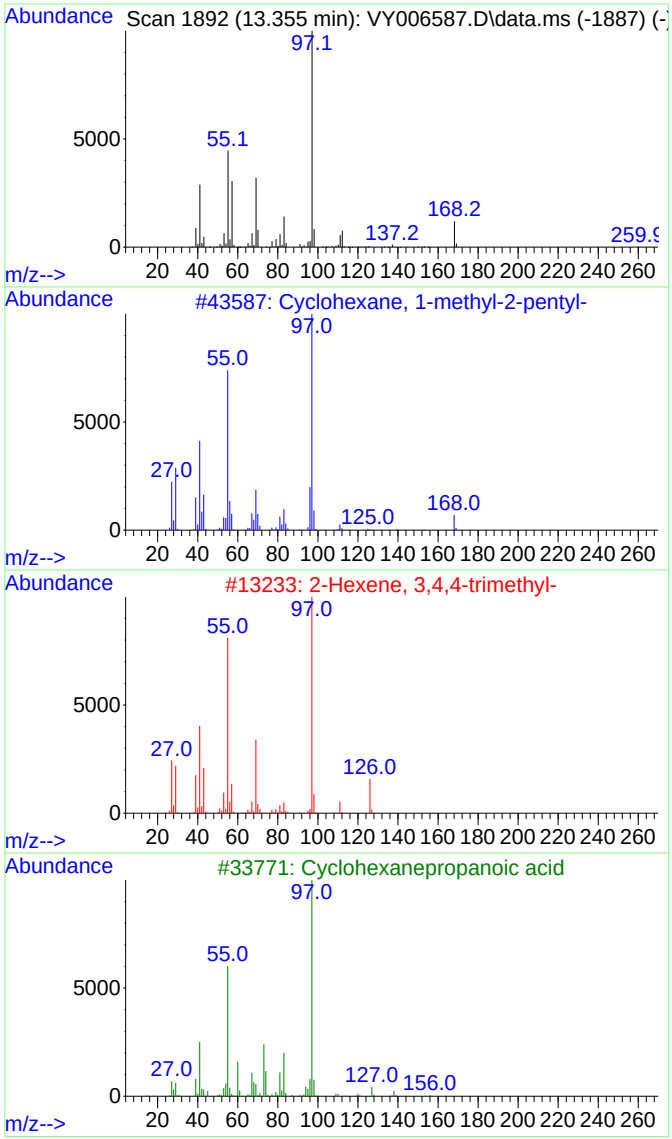
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

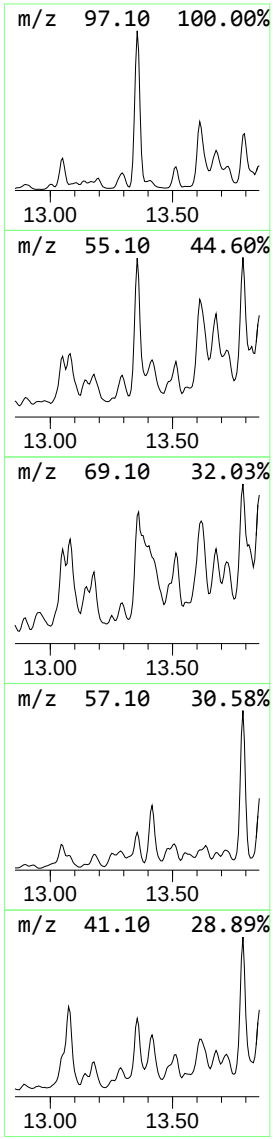
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1-methyl-2-pen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.355	57.54 ug/l	3524180	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	Cyclohexanepropanoic acid	156	C9H16O2	000701-97-3	64
4	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	64
5	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64





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

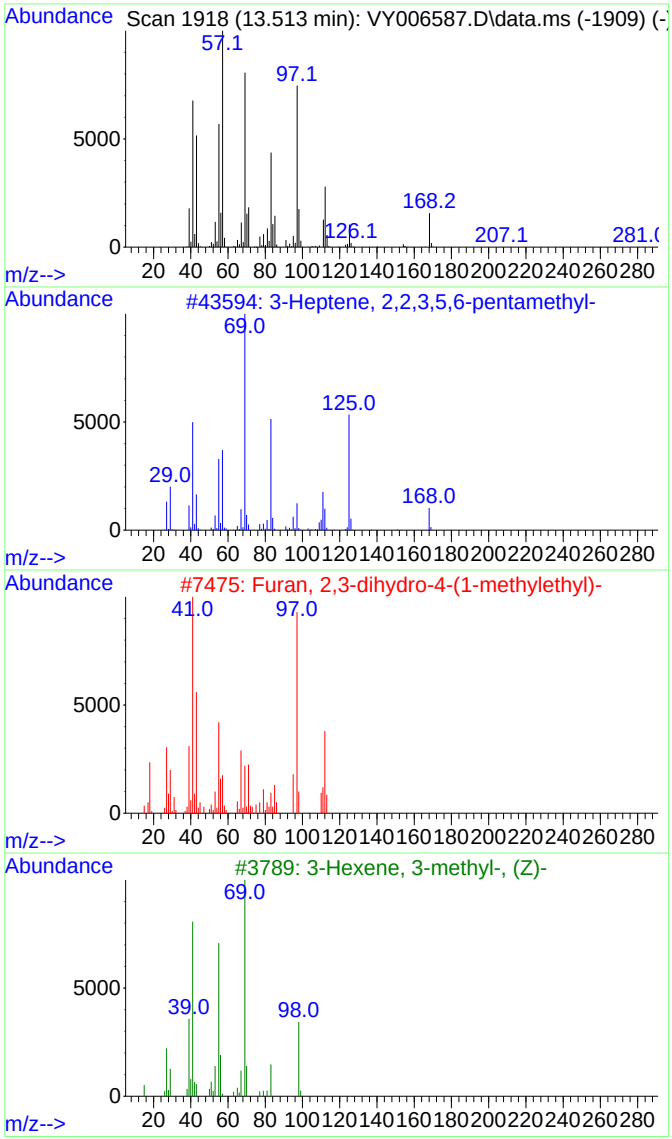
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

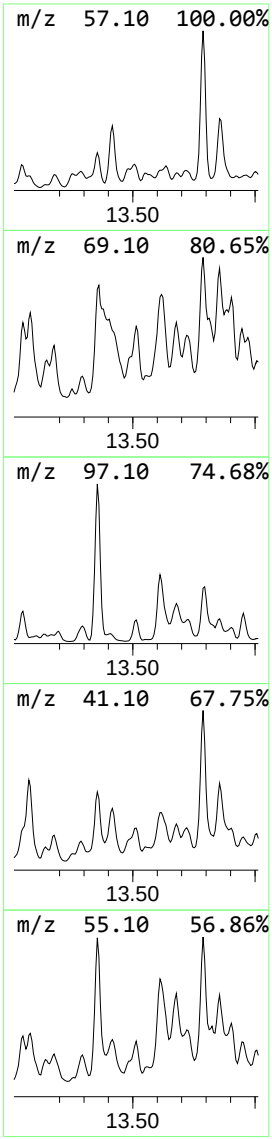
****

Peak Number 4 unknown13.513 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	31.05 ug/l	1901340	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2,2,3,5,6-pentamethyl-	168	C12H24	116164-06-8	46
2	Furan, 2,3-dihydro-4-(1-methylet...	112	C7H12O	034314-84-6	38
3	3-Hexene, 3-methyl-, (Z)-	98	C7H14	004914-89-0	38
4	Formaldehyde, (2-butenyl)methylh...	112	C6H12N2	068661-51-8	30
5	3-Methyl-3-hexene	98	C7H14	003404-65-7	25





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ALS Vial : 21 Sample Multiplier: 1

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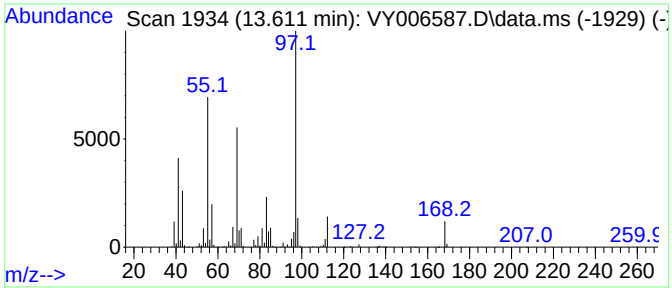
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

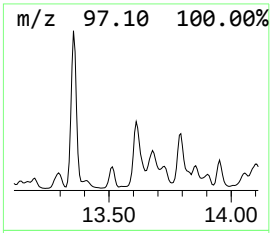
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

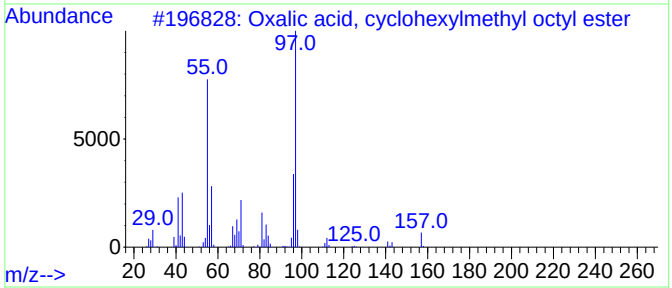
****
Peak Number 5 Oxalic acid, cyclohexylmeth... Concentration Rank 5

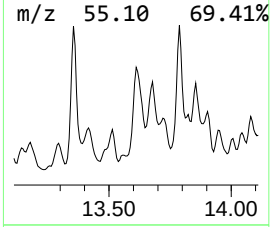
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.611	47.90 ug/l	2933620	1,4-Dichlorobenzene-d4	13.428

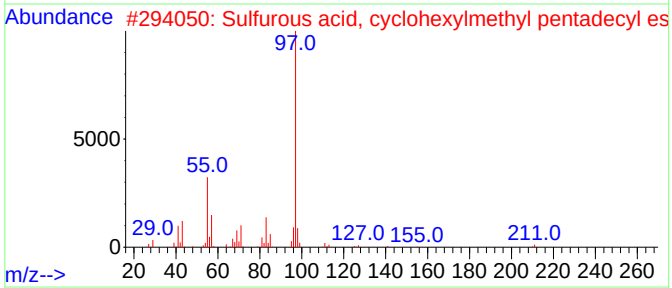
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclohexylmethyl oc...	298	C17H30O4	1000309-68-4	59
2	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	59
3	2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	023758-27-2	58
4	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	53
5	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	53

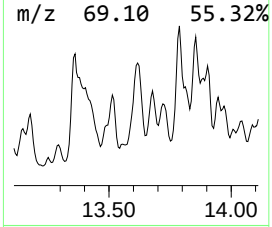


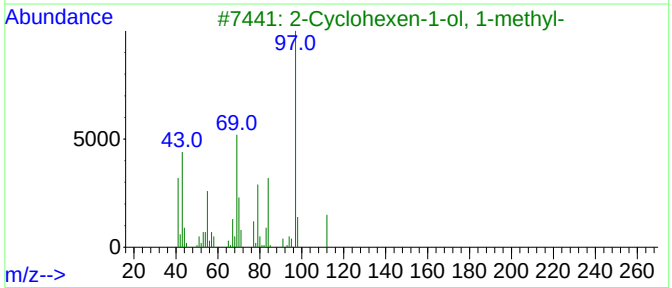


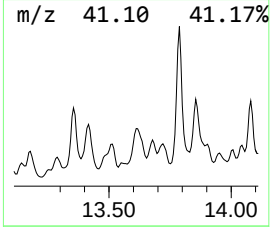


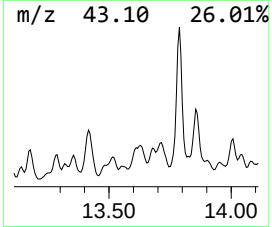












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Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

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

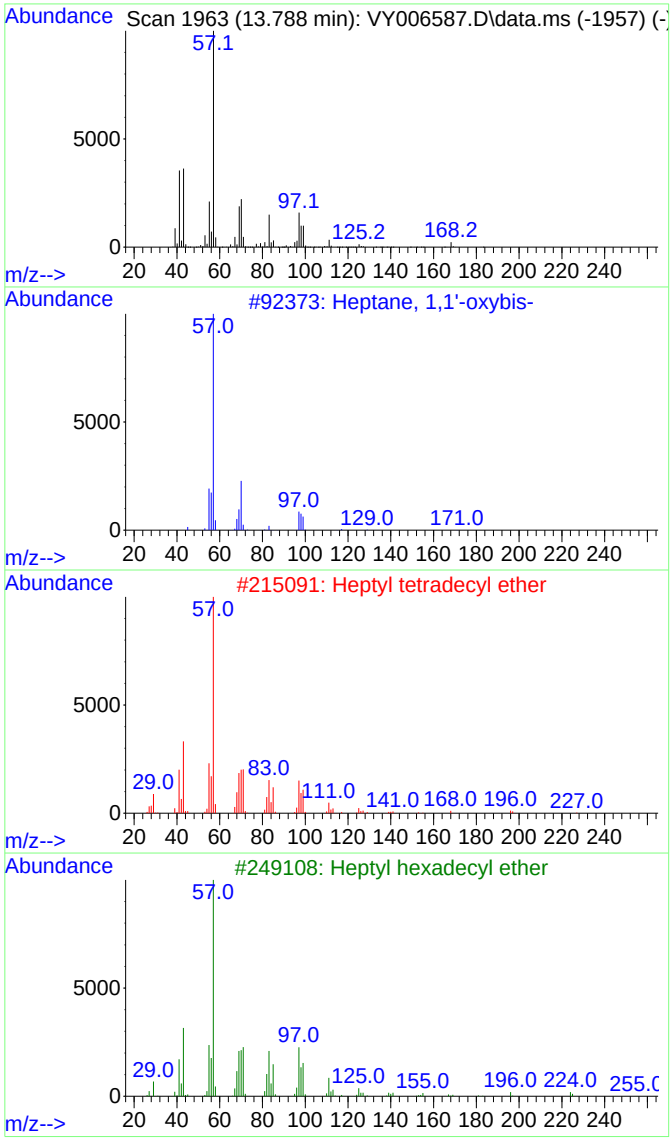
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

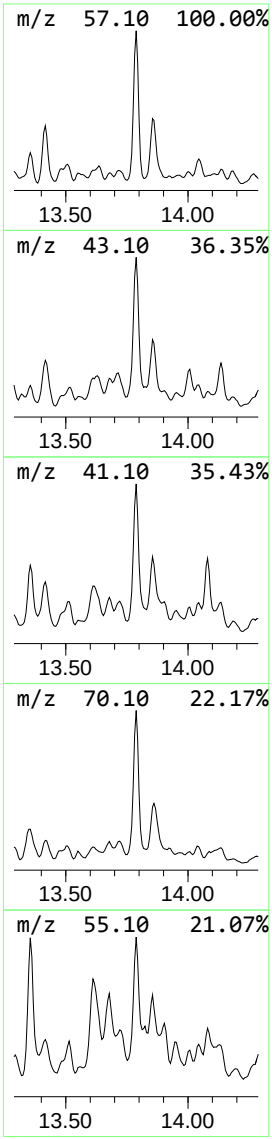
****

Peak Number 6 Heptane, 1,1'-oxybis- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	111.71 ug/l	6841750	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	56
2	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	56
3	Heptyl hexadecyl ether	340	C23H48O	1000406-39-4	56
4	Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	45
5	Heptane, 3-ethyl-	128	C9H20	015869-80-4	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

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

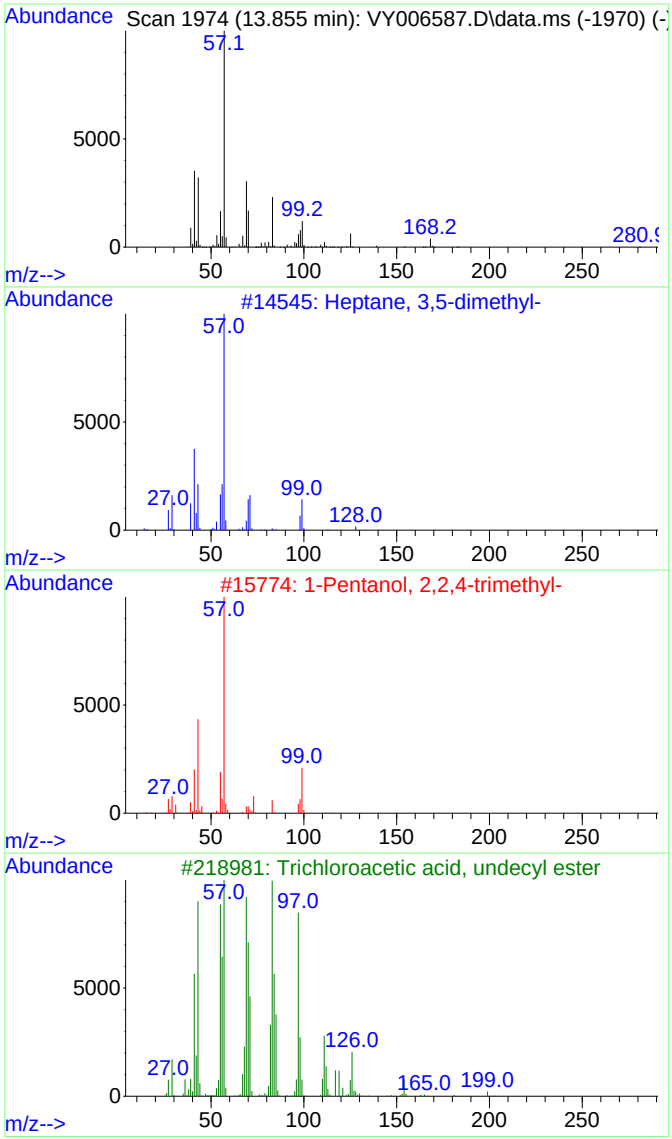
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

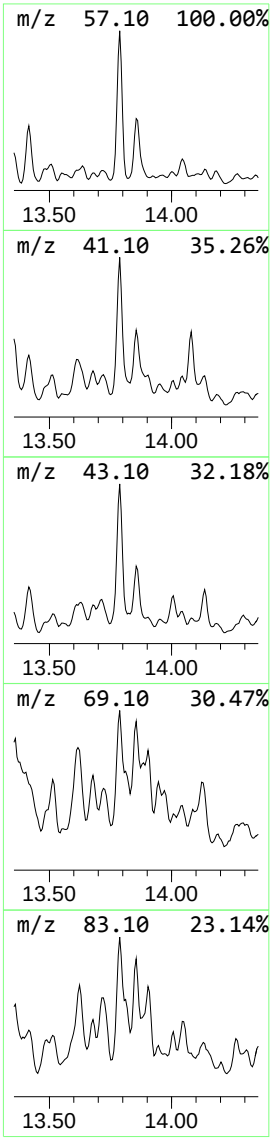
****

Peak Number 7 unknown13.855 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.855	38.03 ug/l	2328990	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38
2	1-Pentanol, 2,2,4-trimethyl-	130	C8H18O	000123-44-4	38
3	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	37
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	28
5	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

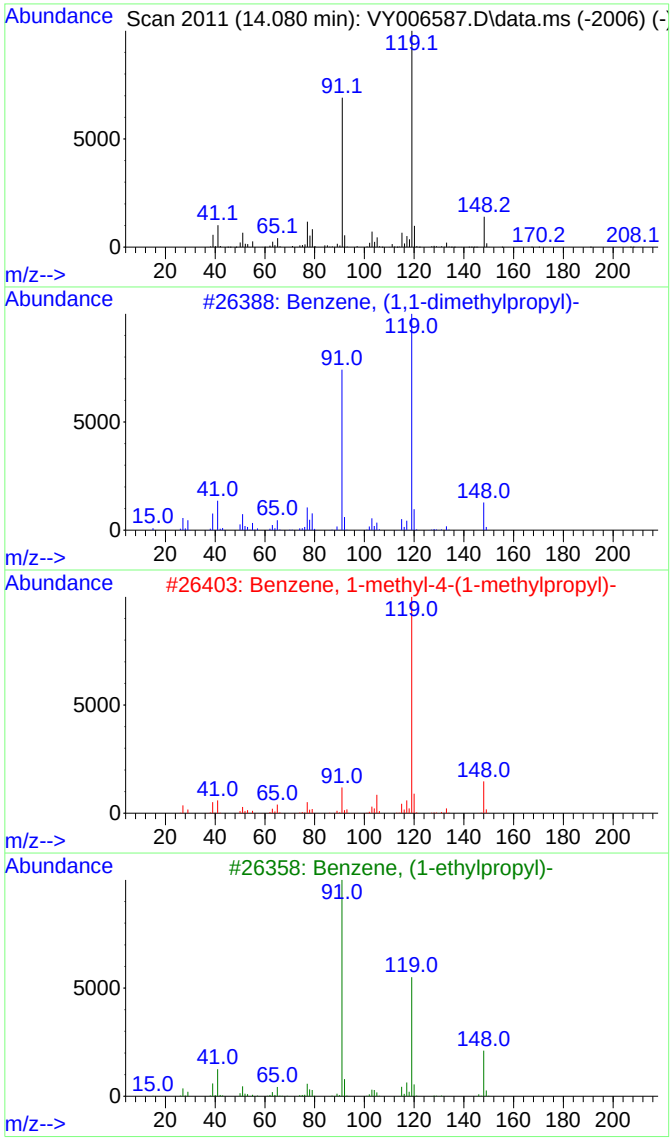
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

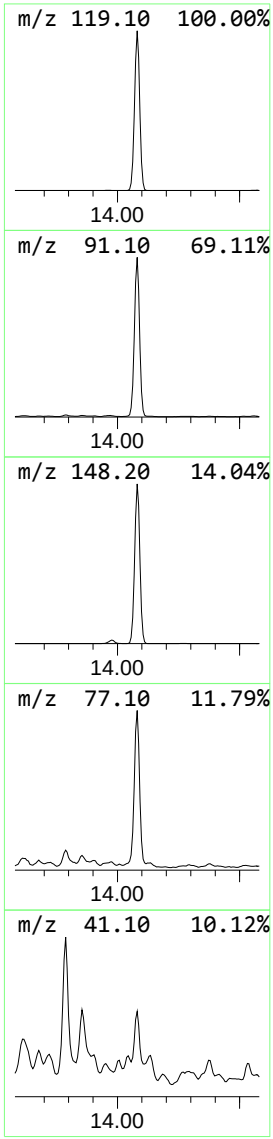
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (1,1-dimethylpropyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	96.86 ug/l	5932400	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	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

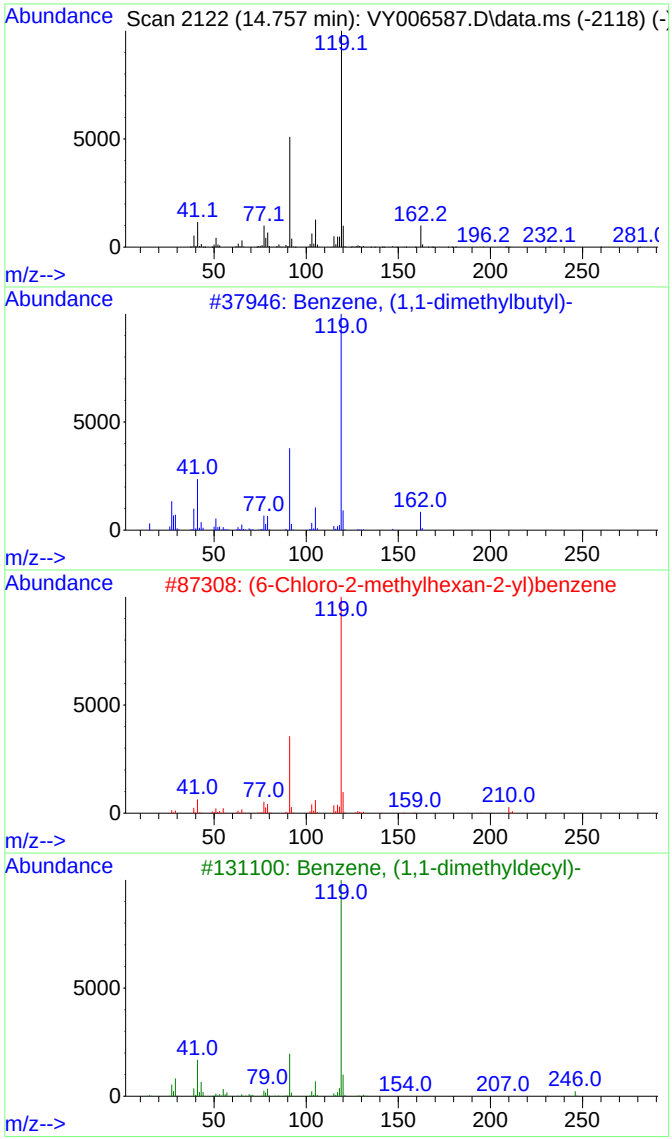
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

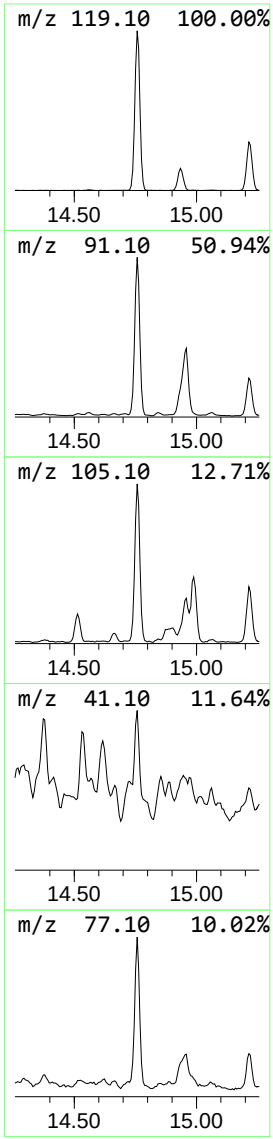
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1,1-dimethylbutyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	39.48 ug/l	2418160	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	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	90
3	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	72
4	Benzene, tert-butyl-	134	C10H14	000098-06-6	72
5	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	72





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Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
Operator : SY/MD
Sample : M4427-04
Misc : 4.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

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

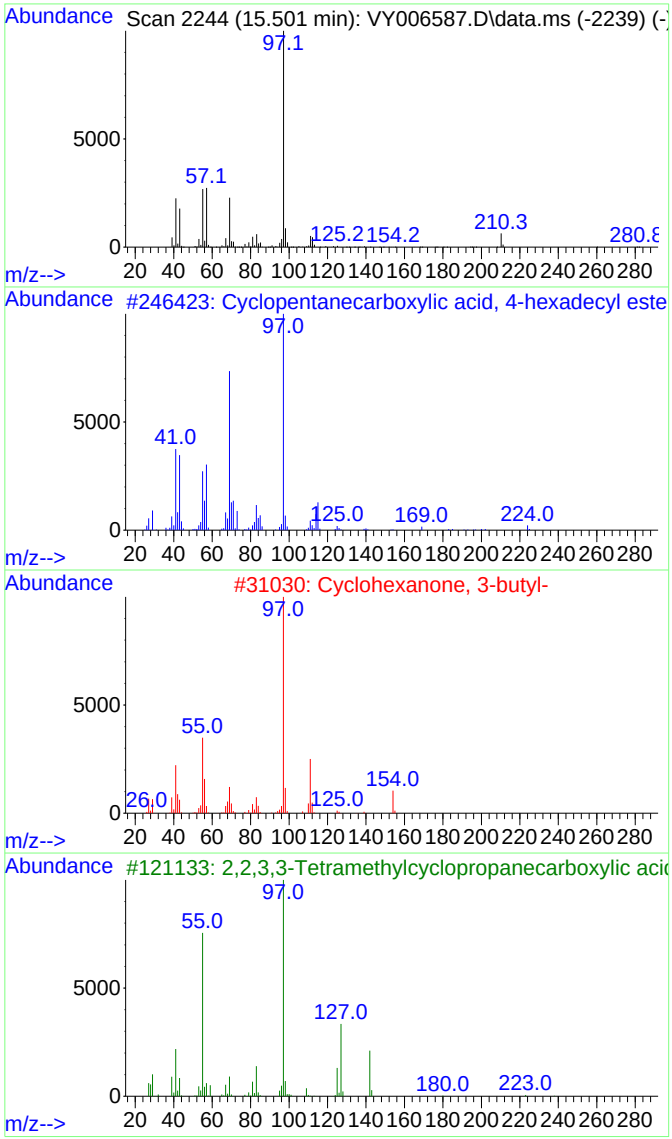
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

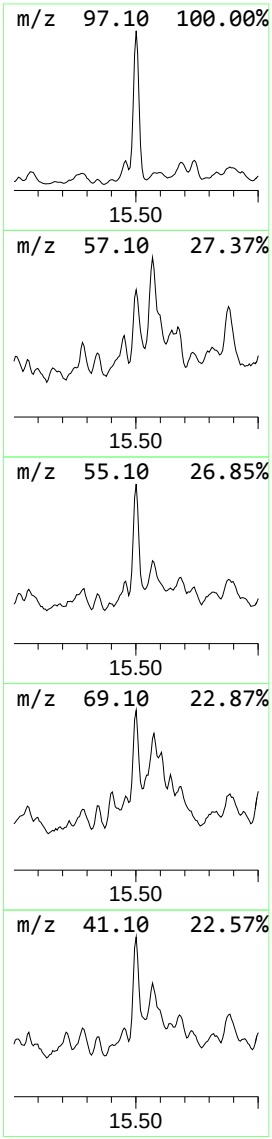
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentanecarboxylic acid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	40.25 ug/l	2465400	1,4-Dichlorobenzene-d4	13.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	78
2	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	72
3	2,2,3,3-Tetramethylcyclopropanec...	238	C15H26O2	1010221-97-5	64
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	64
5	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006587.D
Acq On : 02 Nov 2021 19:23
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MSVOA_Y
ClientSampleId :
FDR-BH-4-20211029-7.5-8M

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Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Heptene, 4-pr...	12.245	27.8	ug/l	402613	3	11.496	723899	50.0
2-Propyl-1-pent...	12.392	60.2	ug/l	871075	3	11.496	723899	50.0
Cyclohexane, 1-...	13.355	57.5	ug/l	3524180	4	13.428	3062240	50.0
unknown13.513	13.513	31.1	ug/l	1901340	4	13.428	3062240	50.0
Oxalic acid, cy...	13.611	47.9	ug/l	2933620	4	13.428	3062240	50.0
Heptane, 1,1'-o...	13.788	111.7	ug/l	6841750	4	13.428	3062240	50.0
unknown13.855	13.855	38.0	ug/l	2328990	4	13.428	3062240	50.0
Benzene, (1,1-d...	14.080	96.9	ug/l	5932400	4	13.428	3062240	50.0
Benzene, (1,1-d...	14.757	39.5	ug/l	2418160	4	13.428	3062240	50.0
Cyclopentanecar...	15.501	40.3	ug/l	2465400	4	13.428	3062240	50.0