LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY101024\
Data File : VY019852.D
Acq On : 10 Oct 2024 14:30
Operator : SY/MD
Sample : P4364-03
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01-4.25-4.83

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\82Y100924S.M
Title : SW846 8260

Signal : TIC: VY019852.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.080	49	59	60	rBV3	4588	9728	12.92%	2.251%
2	2.178	73	75	76	rBV2	1589	1179	1.57%	0.273%
3	2.233	82	84	86	rBV3	1793	2211	2.94%	0.512%
4	2.562	136	138	140	rBV	1330	1049	1.39%	0.243%
5	2.611	142	146	148	rVV3	1714	1844	2.45%	0.427%
6	2.696	158	160	161	rBV	1370	1164	1.55%	0.269%
7	3.111	225	228	232	rBV3	1292	1603	2.13%	0.371%
8	3.507	290	293	294	rVB	1184	1046	1.39%	0.242%
9	3.525	294	296	300	rBV2	881	1489	1.98%	0.345%
10	3.635	310	314	317	rBV3	1249	1561	2.07%	0.361%
11	4.232	409	412	417	rVB4	782	1383	1.84%	0.320%
12	4.318	424	426	429	rVB2	1238	1235	1.64%	0.286%
13	4.360	429	433	436	rVV3	924	1223	1.62%	0.283%
14	4.409	439	441	443	rVB2	1141	1176	1.56%	0.272%
15	4.586	466	470	473	rBV4	957	1519	2.02%	0.351%
16	4.622	473	476	479	rVV3	1049	1348	1.79%	0.312%
17	4.671	479	484	487	rBV3	574	1087	1.44%	0.252%
18	4.793	501	504	507	rBV2	1163	1160	1.54%	0.268%
19	5.647	641	644	650	rVB2	1180	1279	1.70%	0.296%
20	5.775	662	665	668	rBV3	797	1107	1.47%	0.256%
21	5.890	680	684	687	rBV2	812	1235	1.64%	0.286%
22	6.378	762	764	767	rBV	975	1194	1.59%	0.276%
23	6.500	780	784	787	rBV4	775	1384	1.84%	0.320%
24	6.890	838	848	852	rBV3	3897	11884	15.78%	2.750%
25	7.469	940	943	945	rBV2	883	1050	1.39%	0.243%
26	7.640	964	971	977	rBV4	9829	25035	33.25%	5.793%
27	7.713	977	983	992	rVB2	18143	42381	56.29%	9.806%
28	8.055	1030	1039	1048	rBV5	12145	35693	47.41%	8.259%
29	8.457	1102	1105	1108	rVB	1359	1443	1.92%	0.334%
30	8.616	1124	1131	1140	rBV	27436	56776	75.41%	13.137%
31	9.067	1202	1205	1208	rBV2	878	1471	1.95%	0.340%
32	9.103	1208	1211	1215	rVB2	1247	1537	2.04%	0.356%
33	9.176	1221	1223	1225	rBV2	1027	1290	1.71%	0.298%
34	9.231	1231	1232	1237	rVV2	1139	1102	1.46%	0.255%
35	9.292	1240	1242	1246	rVB	1349	1476	1.96%	0.342%
36	9.634	1295	1298	1303	rVB3	1067	1562	2.07%	0.361%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
SB-01-4.25-4.83

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Title : SW846 8260

37	10.109	1368	1376	1384	rBV	40268	75292	100.00%	17.422%
38	10.335	1409	1413	1416	rBV3	968	1253	1.66%	0.290%
39	10.835	1492	1495	1497	rBV2	969	1473	1.96%	0.341%
40	10.877	1498	1502	1508	rVB3	1559	2546	3.38%	0.589%
41	11.414	1582	1590	1599	rBV	29885	53920	71.61%	12.476%
42	11.719	1636	1640	1641	rBV	865	1025	1.36%	0.237%
43	11.944	1674	1677	1679	rBV3	907	1028	1.37%	0.238%
44	12.036	1687	1692	1693	rBV	1069	1119	1.49%	0.259%
45	12.121	1702	1706	1710	rBV2	1079	1937	2.57%	0.448%
46	12.408	1747	1753	1759	rVB4	14190	25678	34.10%	5.942%
47	13.346	1902	1907	1911	rVB3	7941	11835	15.72%	2.738%
48	13.718	1964	1968	1970	rBV2	845	1240	1.65%	0.287%
49	13.877	1989	1994	1995	rBV3	1544	1766	2.35%	0.409%
50	14.212	2046	2049	2051	rBV3	946	1217	1.62%	0.282%
51	14.395	2077	2079	2082	rBV3	912	1043	1.39%	0.241%
52	15.078	2186	2191	2193	rBV3	1221	1705	2.26%	0.395%
53	15.145	2198	2202	2203	rVB3	2058	1820	2.42%	0.421%
54	15.188	2203	2209	2213	rBV2	1037	1952	2.59%	0.452%
55	15.291	2223	2226	2227	rBV2	765	1044	1.39%	0.242%
56	15.383	2236	2241	2244	rVB6	1093	1917	2.55%	0.444%
57	15.425	2244	2248	2250	rBV4	1178	1605	2.13%	0.371%
58	15.755	2299	2302	2306	rBV3	910	1503	2.00%	0.348%
59	15.803	2306	2310	2315	rVB5	1168	1917	2.55%	0.444%
60	16.029	2343	2347	2349	rVB3	1085	1410	1.87%	0.326%
61	16.059	2349	2352	2353	rBV	1171	1099	1.46%	0.254%
62	16.108	2357	2360	2364	rVB4	838	1160	1.54%	0.268%
63	16.163	2366	2369	2371	rBV4	1538	1875	2.49%	0.434%
64	16.303	2387	2392	2393	rBV3	1205	1838	2.44%	0.425%
65	16.474	2418	2420	2423	rBV4	1024	1198	1.59%	0.277%
66	16.529	2427	2429	2432	rVB2	1253	1035	1.37%	0.239%
67	16.565	2432	2435	2438	rBV3	1955	2059	2.73%	0.476%
68	16.632	2445	2446	2449	rVB2	1439	1189	1.58%	0.275%
69	16.718	2458	2460	2464	rVB5	1111	1575	2.09%	0.364%

Sum of corrected areas: 432177

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ALS Vial : 13 Sample Multiplier: 1

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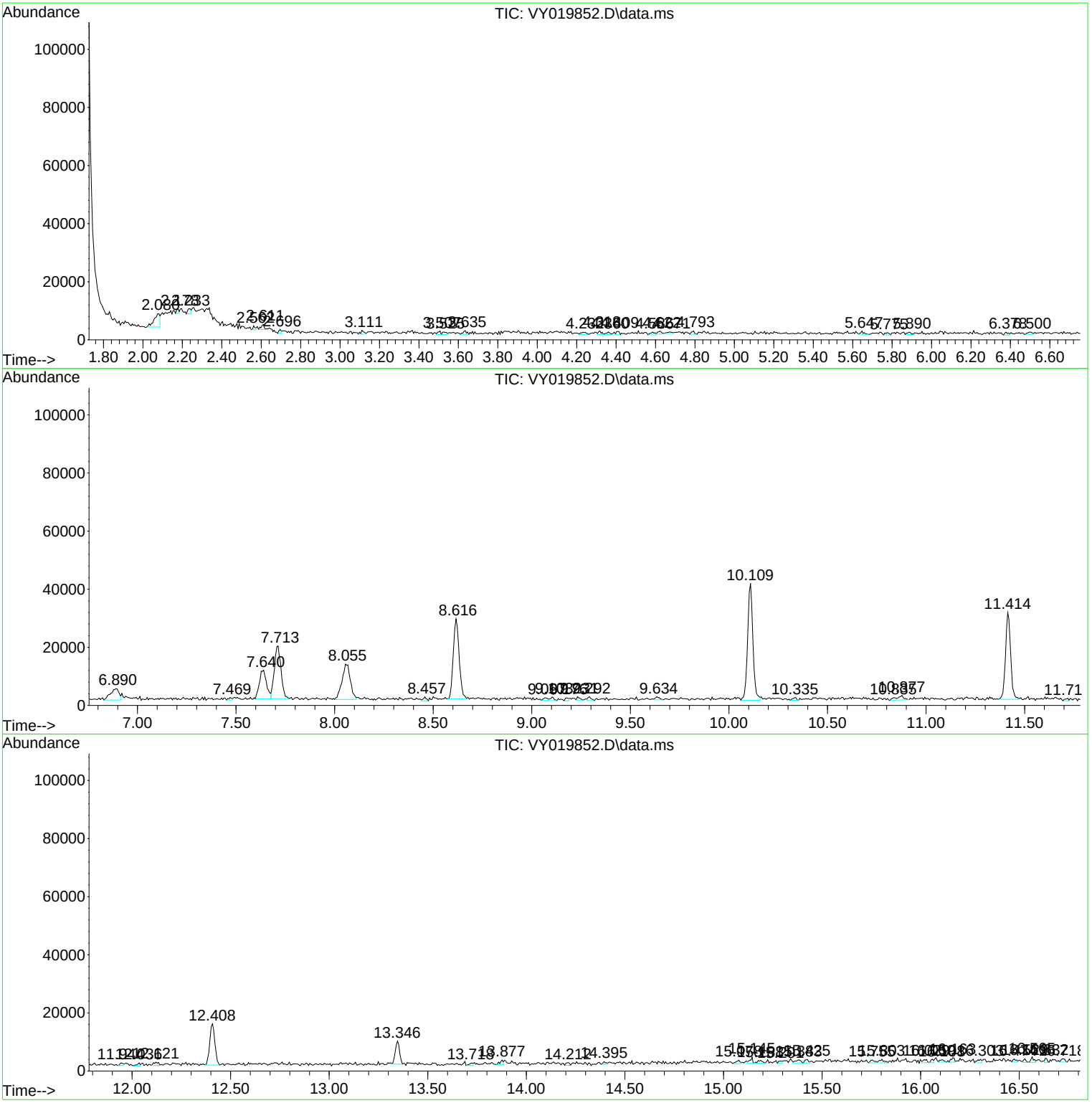
MSVOA_Y
ClientSampleId :
SB-01-4.25-4.83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY101024\
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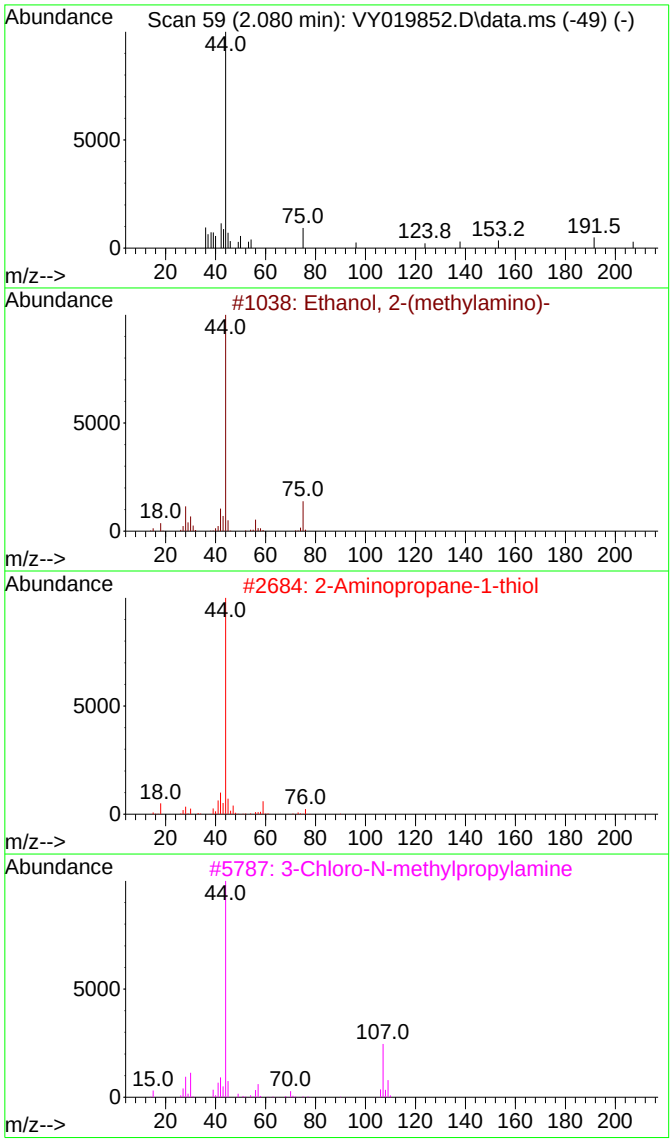
Quant Title : SW846 8260

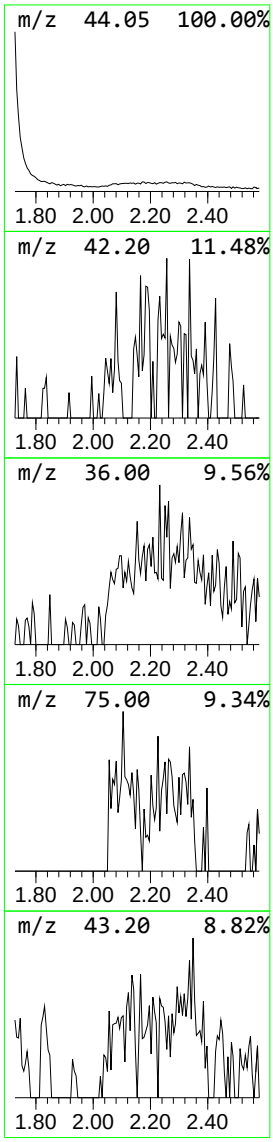
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(methylamino)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.080	11.48 ug/l	9728	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(methylamino)-	75	C3H9NO	000109-83-1	59
2	2-Aminopropane-1-thiol	91	C3H9NS	010229-29-5	9
3	3-Chloro-N-methylpropylamine	107	C4H10ClN	065232-62-4	9
4	Imidazole, 2-amino-5-[(2-carboxy...	153	C6H7N3O2	1000116-74-7	5
5	1-Propanol, 3-amino-	75	C3H9NO	000156-87-6	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY101024\
Data File : VY019852.D
Acq On : 10 Oct 2024 14:30
Operator : SY/MD
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01-4.25-4.83

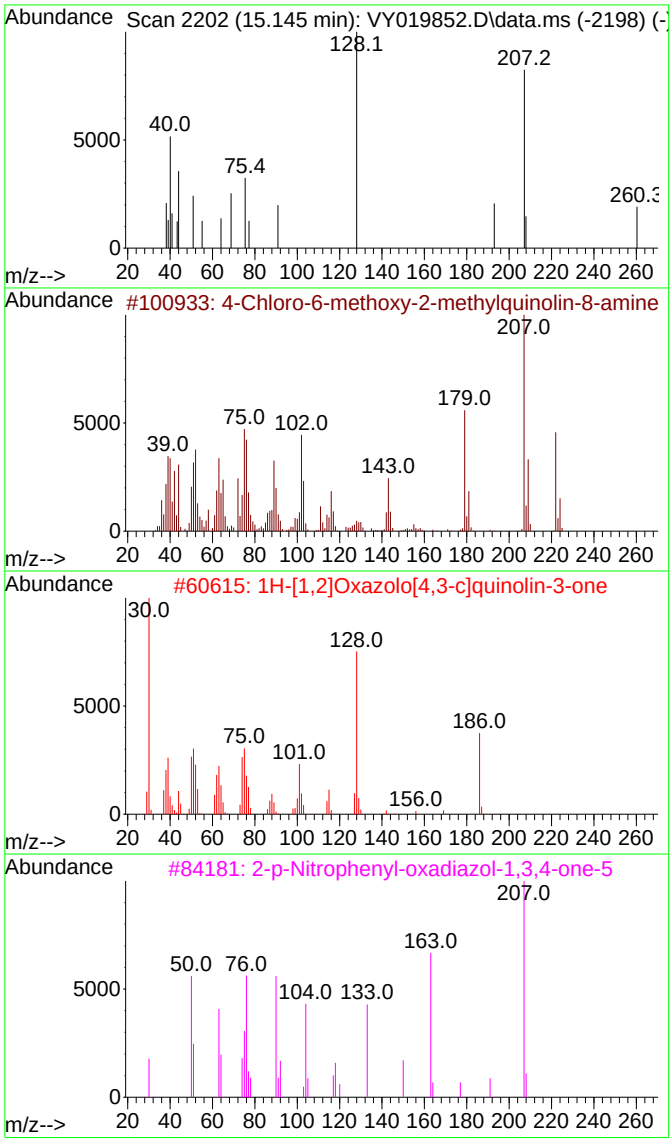
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

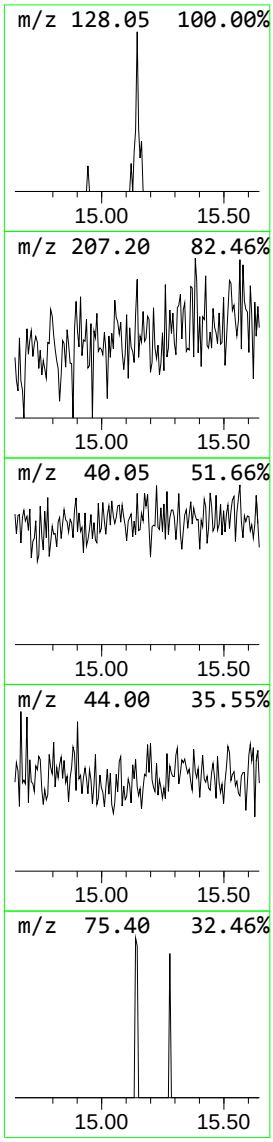
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown15.145 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	7.69 ug/l	1820	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-methoxy-2-methylquino...	222	C11H11ClN2O	1000411-05-4	23
2	1H-[1,2]Oxazolo[4,3-c]quinolin-3...	186	C10H6N2O2	1000443-27-0	23
3	2-p-Nitrophenyl-oxadiazol-1,3,4-...	207	C8H5N3O4	1000147-64-6	22
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	16
5	3-Amino-7-nitro-1,2,4-benzotriaz...	207	C7H5N5O3	1010256-54-1	16





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Data File : VY019852.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01-4.25-4.83

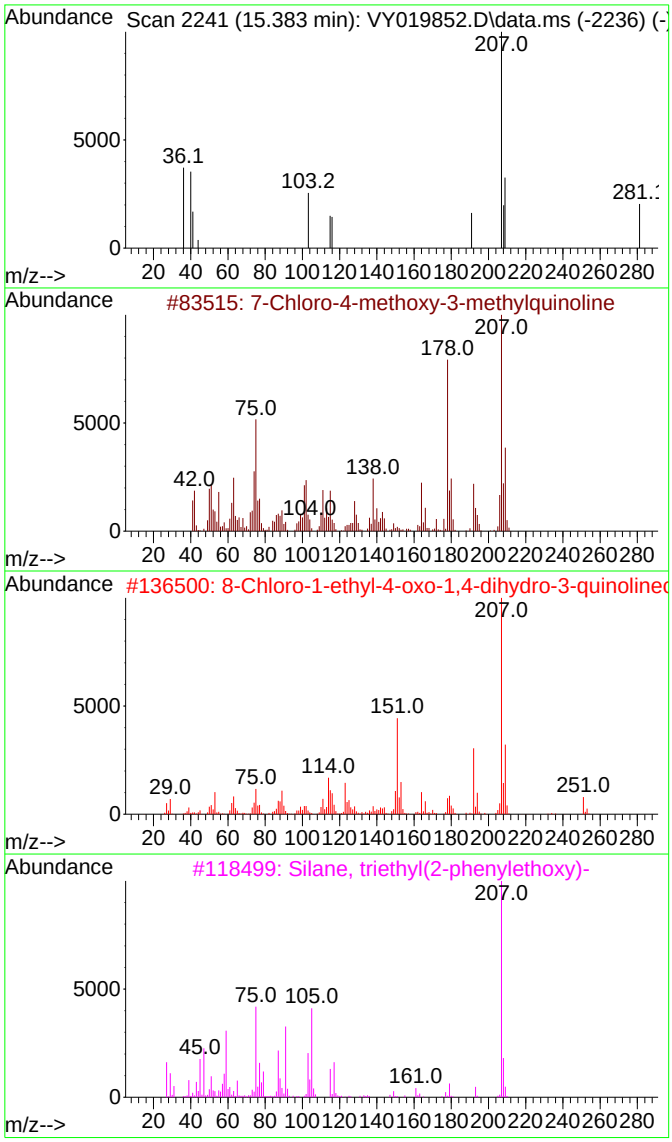
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

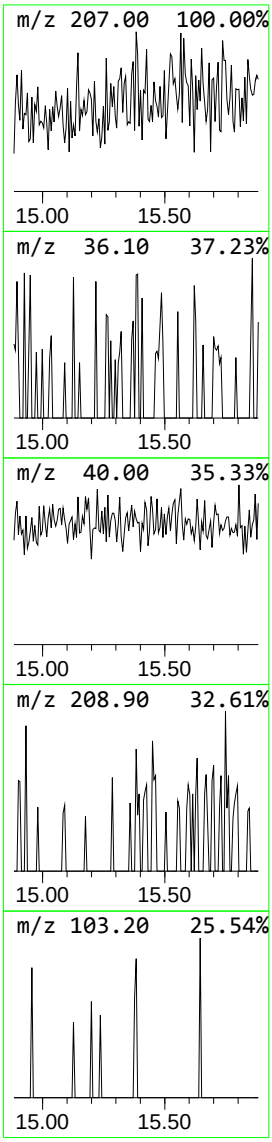
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown15.383 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.383	8.10 ug/l	1917	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Chloro-4-methoxy-3-methylquino...	207	C11H10ClNO	1000213-52-2	40
2	8-Chloro-1-ethyl-4-oxo-1,4-dihyd...	251	C12H10ClNO3	051395-55-2	33
3	Silane, triethyl(2-phenylethoxy)-	236	C14H24OSi	014629-62-0	28
4	Quinoline, 4-chloro-6-methoxy-2-...	207	C11H10ClNO	050593-73-2	9
5	7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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Quant Title : SW846 8260

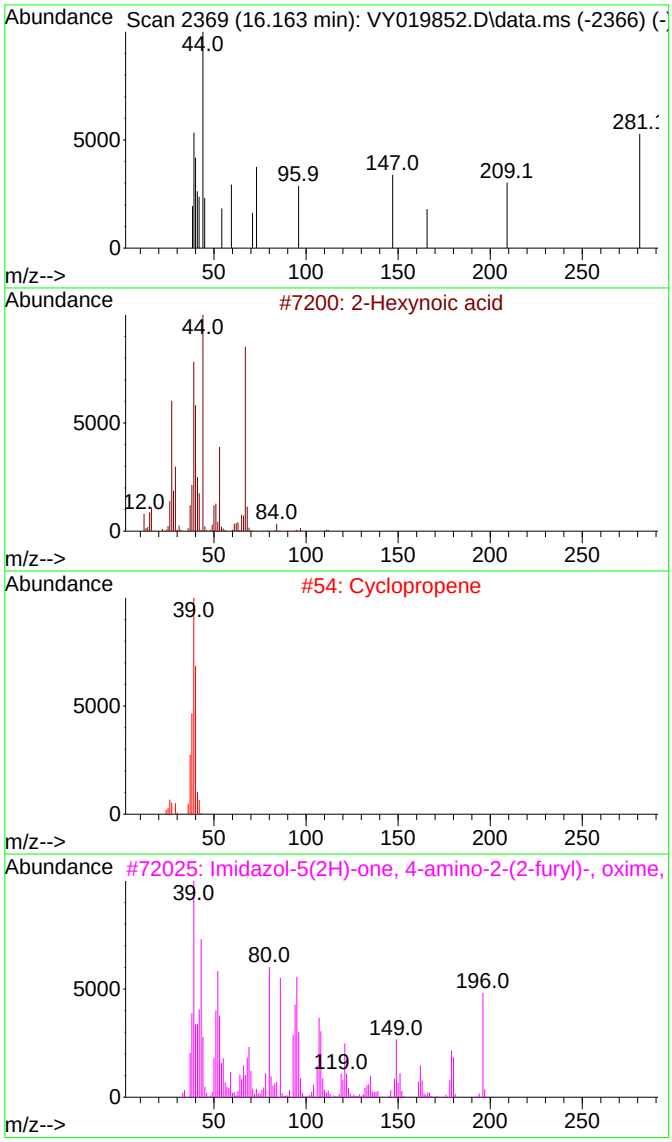
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

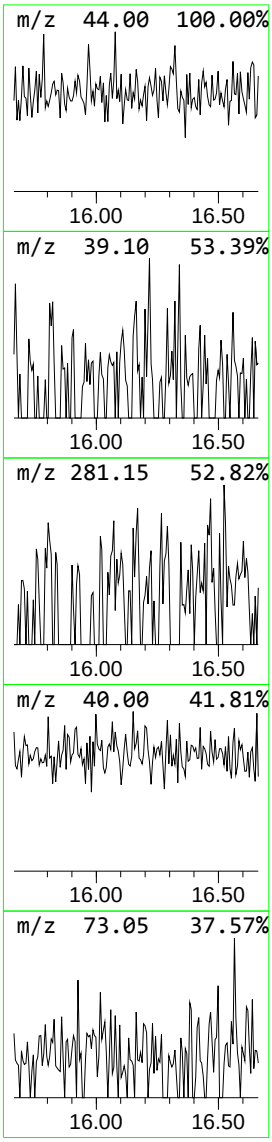
****

Peak Number 8 unknown16.163 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.163	7.92 ug/l	1875	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexynoic acid	112	C6H8O2	000764-33-0	17
2	Cyclopropene	40	C3H4	002781-85-3	9
3	Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	9
4	Dodecamethylene imine	183	C12H25N	1000430-67-9	9
5	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	9





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Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-01-4.25-4.83

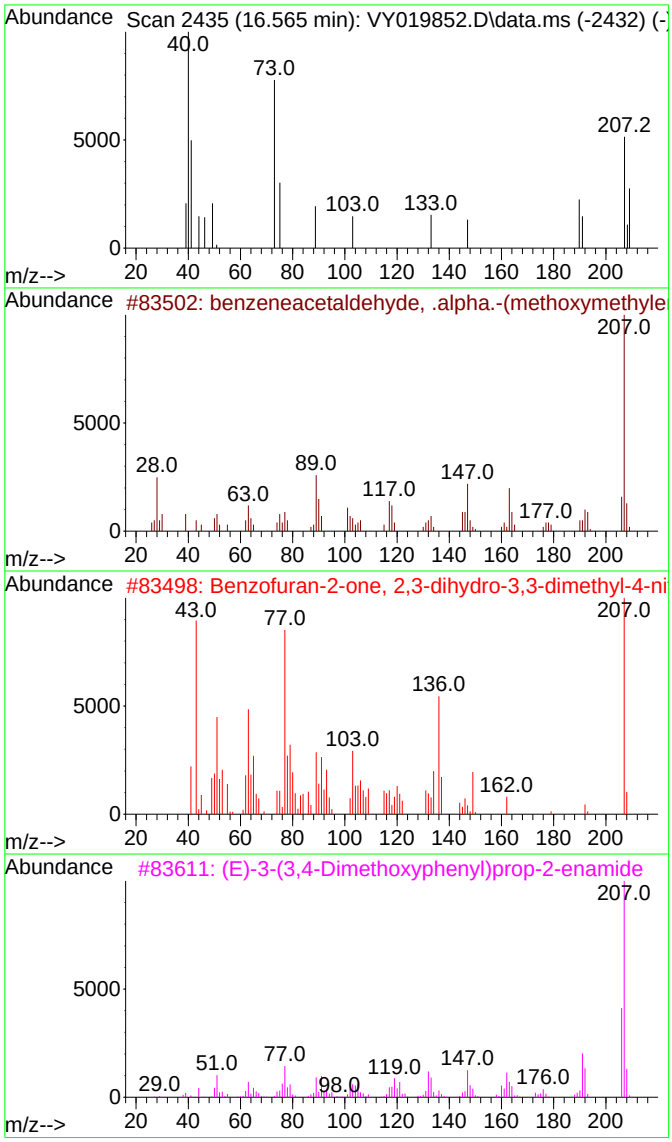
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

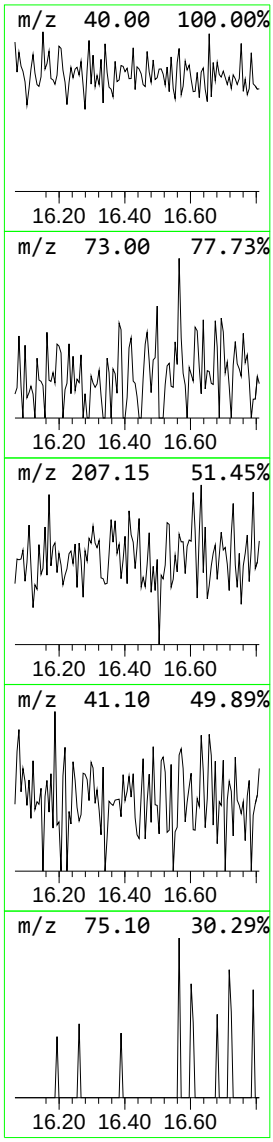
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.565 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.565	8.70 ug/l	2059	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	benzeneacetaldehyde, .alpha.-(me...	207	C10H9NO4	1000396-10-6	22
2	Benzofuran-2-one, 2,3-dihydro-3,...	207	C10H9NO4	1000129-53-4	14
3	(E)-3-(3,4-Dimethoxyphenyl)prop-...	207	C11H13NO3	130973-10-3	10
4	2-(4-Methyl-5-sulfanyl-4H-1,2,4-...	207	C9H9N3OS	1000476-79-6	9
5	Indole-2-one, 2,3-dihydro-N-hydr...	207	C11H13NO3	1010129-52-1	9





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
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
Ethanol, 2-(met...	2.080	11.5	ug/l	9728	1	7.707	42381	50.0
unknown15.145	15.145	7.7	ug/l	1820	4	13.347	11835	50.0
unknown15.383	15.383	8.1	ug/l	1917	4	13.347	11835	50.0
unknown16.163	16.163	7.9	ug/l	1875	4	13.347	11835	50.0
unknown16.565	16.565	8.7	ug/l	2059	4	13.347	11835	50.0