LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

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_X\Method\82X100322W.M
Title : SW846 8260

Signal : TIC: VX031850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	26	33	48	rBV	79409	324413	50.79%	3.211%
2	5.385	692	705	720	rBV2	79523	231113	36.19%	2.288%
3	5.550	720	732	748	rVB	78911	218057	34.14%	2.158%
4	5.952	788	798	816	rBV	76860	206734	32.37%	2.046%
5	6.763	922	931	946	rVB	107470	256393	40.14%	2.538%
6	8.647	1234	1240	1249	rBV	380786	600276	93.99%	5.942%
7	10.055	1465	1471	1479	rBV	264464	352474	55.19%	3.489%
8	10.281	1503	1508	1517	rBV7	4142	9321	1.46%	0.092%
9	10.592	1551	1559	1565	rBV7	3101	8059	1.26%	0.080%
10	10.964	1614	1620	1624	rBV	7498	9335	1.46%	0.092%
11	11.079	1634	1639	1645	rBV	300098	383693	60.07%	3.798%
12	11.220	1652	1662	1668	rBV3	6750	13294	2.08%	0.132%
13	11.616	1721	1727	1734	rBV4	7902	14230	2.23%	0.141%
14	11.713	1739	1743	1746	rBV3	7395	8256	1.29%	0.082%
15	11.860	1759	1767	1769	rBV7	3886	8185	1.28%	0.081%
16	11.890	1769	1772	1776	rVB	11056	14770	2.31%	0.146%
17	12.024	1788	1794	1800	rBV	319705	410438	64.26%	4.063%
18	12.177	1814	1819	1824	rVB	25338	35550	5.57%	0.352%
19	12.244	1824	1830	1837	rBV2	513923	638690	100.00%	6.322%
20	12.311	1837	1841	1848	rVB	34818	49840	7.80%	0.493%
21	12.408	1850	1857	1861	rVV	22663	31608	4.95%	0.313%
22	12.610	1887	1890	1893	rBV	16429	20682	3.24%	0.205%
23	12.646	1893	1896	1900	rVB	90979	104690	16.39%	1.036%
24	12.701	1900	1905	1912	rVB	219315	301361	47.18%	2.983%
25	12.756	1912	1914	1920	rVB	11687	15024	2.35%	0.149%
26	12.841	1920	1928	1933	rVB2	32980	62116	9.73%	0.615%
27	12.902	1933	1938	1939	rBV	19023	24724	3.87%	0.245%
28	12.921	1939	1941	1946	rVB	28117	31790	4.98%	0.315%
29	12.981	1946	1951	1954	rBV3	11530	15873	2.49%	0.157%
30	13.030	1954	1959	1965	rVB3	53465	78385	12.27%	0.776%
31	13.097	1965	1970	1973	rBV	20795	32653	5.11%	0.323%
32	13.134	1973	1976	1980	rBV	50282	57972	9.08%	0.574%
33	13.170	1980	1982	1983	rVV2	13031	11417	1.79%	0.113%
34	13.195	1983	1986	1991	rVB	37222	47182	7.39%	0.467%
35	13.256	1991	1996	1998	rBV2	16174	24509	3.84%	0.243%
36	13.292	1998	2002	2008	rVB	343863	412228	64.54%	4.080%

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ClientSampleId :
MW-07

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	13.347	2008	2011	2014	rBV3	28403	35406	5.54%	0.350%
38	13.390	2015	2018	2020	rVV2	16124	23269	3.64%	0.230%
39	13.420	2020	2023	2032	rVB2	43523	74210	11.62%	0.735%
40	13.506	2032	2037	2040	rBV3	24447	36967	5.79%	0.366%
41	13.542	2040	2043	2046	rVV	71944	89041	13.94%	0.881%
42	13.585	2046	2050	2053	rVV2	138264	174969	27.39%	1.732%
43	13.640	2053	2059	2060	rVV2	129169	182879	28.63%	1.810%
44	13.664	2060	2063	2068	rVV	213033	279514	43.76%	2.767%
45	13.750	2072	2077	2081	rBV3	26365	39178	6.13%	0.388%
46	13.798	2081	2085	2089	rBV4	29048	41962	6.57%	0.415%
47	13.853	2089	2094	2099	rVB3	129954	174345	27.30%	1.726%
48	13.926	2099	2106	2110	rBV2	230885	300287	47.02%	2.972%
49	13.969	2110	2113	2117	rVV	90780	120455	18.86%	1.192%
50	14.006	2117	2119	2123	rVB	27339	29950	4.69%	0.296%
51	14.073	2125	2130	2133	rBV	87788	113828	17.82%	1.127%
52	14.103	2133	2135	2138	rVV2	17768	21042	3.29%	0.208%
53	14.134	2138	2140	2142	rVV3	13157	16739	2.62%	0.166%
54	14.164	2142	2145	2147	rVV	20710	24662	3.86%	0.244%
55	14.213	2148	2153	2163	rVV	188763	310687	48.64%	3.075%
56	14.286	2163	2165	2167	rVV	29338	28138	4.41%	0.279%
57	14.323	2167	2171	2175	rVV	125569	164782	25.80%	1.631%
58	14.371	2175	2179	2184	rVV	170652	222548	34.84%	2.203%
59	14.420	2184	2187	2192	rVB	47494	62147	9.73%	0.615%
60	14.481	2192	2197	2202	rBV2	265115	366182	57.33%	3.625%
61	14.524	2202	2204	2210	rVV3	23559	34876	5.46%	0.345%
62	14.615	2210	2219	2225	rVV4	152619	323188	50.60%	3.199%
63	14.676	2225	2229	2233	rVV	91621	127626	19.98%	1.263%
64	14.725	2233	2237	2243	rVV3	43791	69075	10.82%	0.684%
65	14.786	2243	2247	2250	rVV2	72268	127732	20.00%	1.264%
66	14.817	2250	2252	2255	rVV2	77890	103135	16.15%	1.021%
67	14.847	2255	2257	2261	rVV2	56348	68559	10.73%	0.679%
68	14.902	2261	2266	2273	rVV4	52972	127583	19.98%	1.263%
69	14.963	2273	2276	2283	rVB5	26929	60705	9.50%	0.601%
70	15.048	2285	2290	2294	rBV2	31286	44645	6.99%	0.442%
71	15.182	2307	2312	2316	rBV	137392	233708	36.59%	2.313%
72	15.249	2320	2323	2331	rVB6	25818	57011	8.93%	0.564%
73	15.323	2331	2335	2339	rVB5	12787	21053	3.30%	0.208%
74	15.371	2339	2343	2346	rBV3	29446	48116	7.53%	0.476%
75	15.408	2346	2349	2353	rVB3	23060	32943	5.16%	0.326%
76	15.481	2357	2361	2364	rBV2	21445	33309	5.22%	0.330%

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Title : SW846 8260

77	15.524	2364	2368	2373	rVB5	26584	48947	7.66%	0.485%
78	15.609	2379	2382	2387	rVB3	30563	45588	7.14%	0.451%
79	15.743	2397	2404	2408	rBV6	20033	49808	7.80%	0.493%
80	15.810	2410	2415	2418	rVV	51652	87738	13.74%	0.868%
81	15.847	2418	2421	2435	rVB3	47134	95474	14.95%	0.945%
82	15.987	2439	2444	2448	rBV2	27856	44205	6.92%	0.438%
83	16.085	2456	2460	2465	rBV7	10322	19399	3.04%	0.192%
84	16.267	2485	2490	2491	rBV2	14275	22775	3.57%	0.225%
85	16.377	2506	2508	2511	rBV3	5178	6599	1.03%	0.065%
86	16.475	2520	2524	2528	rBV2	10332	17950	2.81%	0.178%
87	16.530	2529	2533	2538	rVV3	16899	40947	6.41%	0.405%
88	16.597	2540	2544	2549	rVV3	27501	54010	8.46%	0.535%
89	16.658	2549	2554	2562	rVB2	31869	57229	8.96%	0.566%

Sum of corrected areas: 10102455

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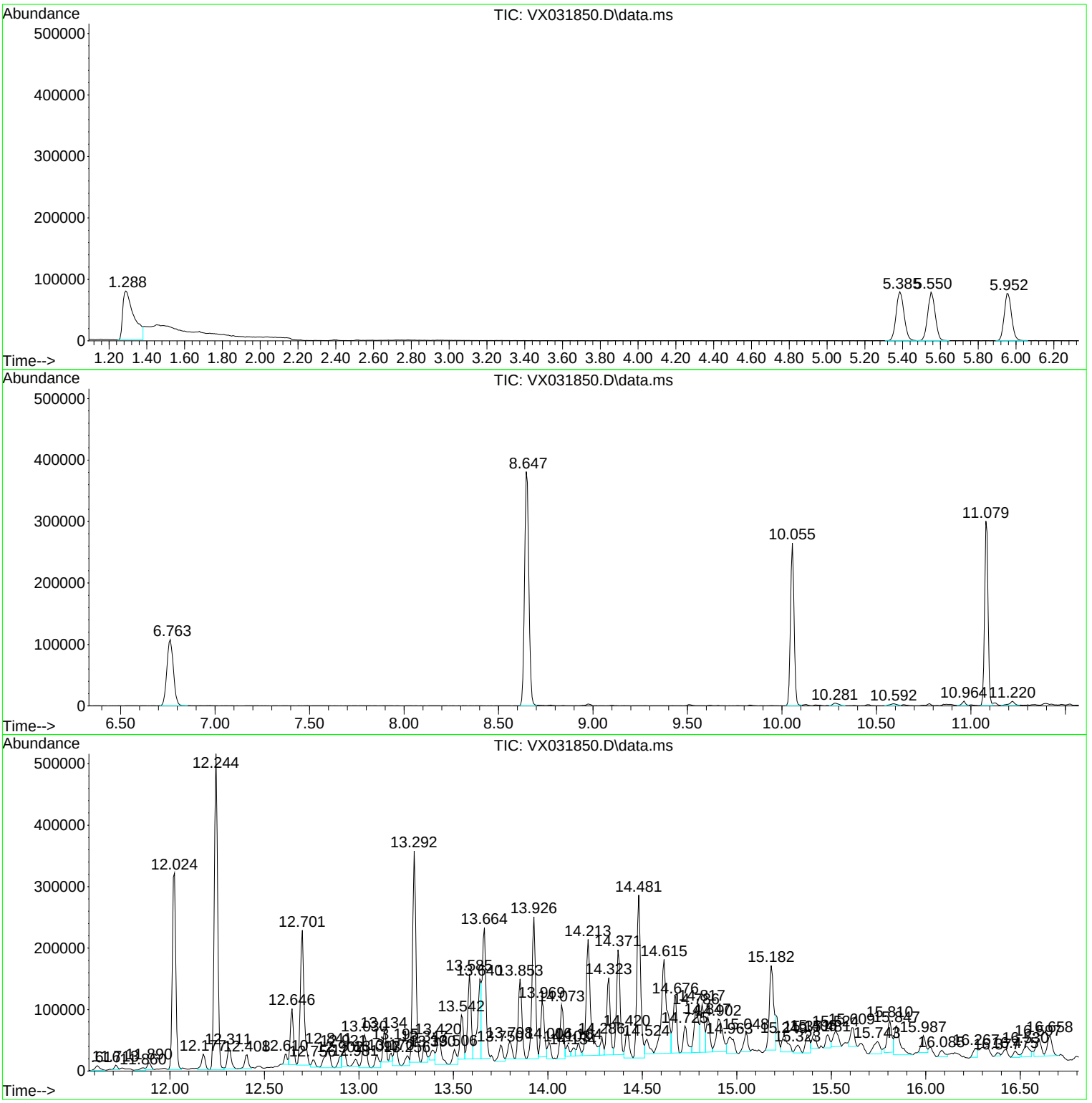
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

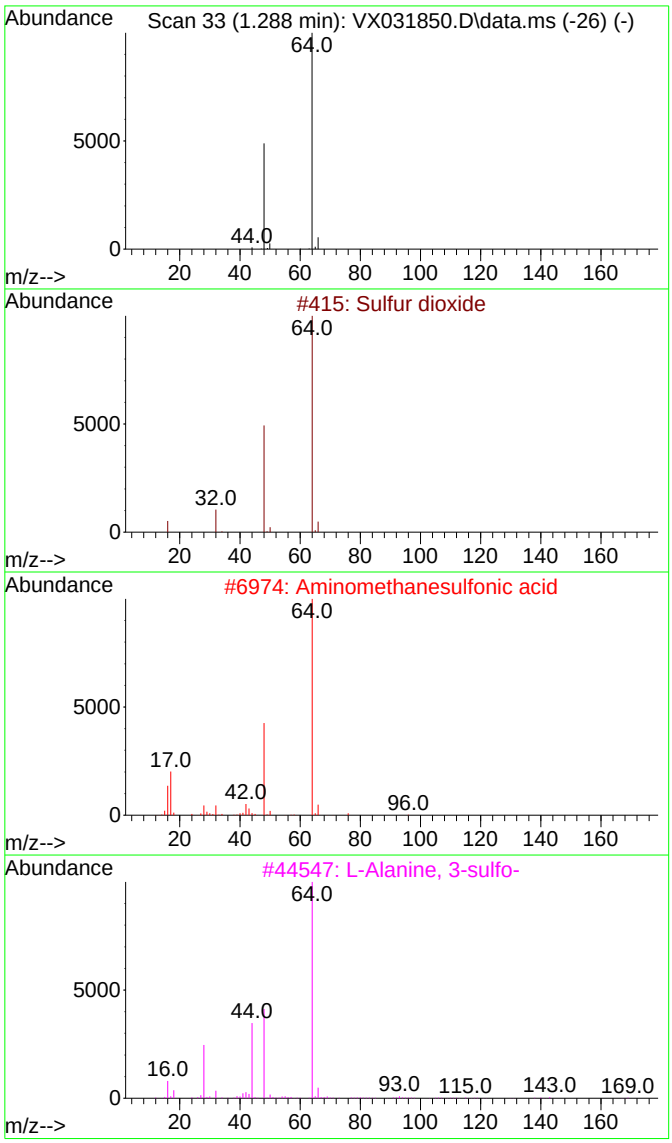
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

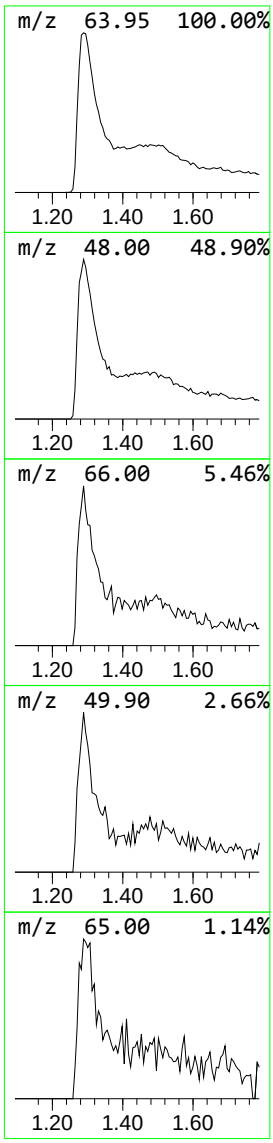
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.288	74.39 ug/l	324413	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument :
MSVOA_X
ClientSampleId :
MW-07

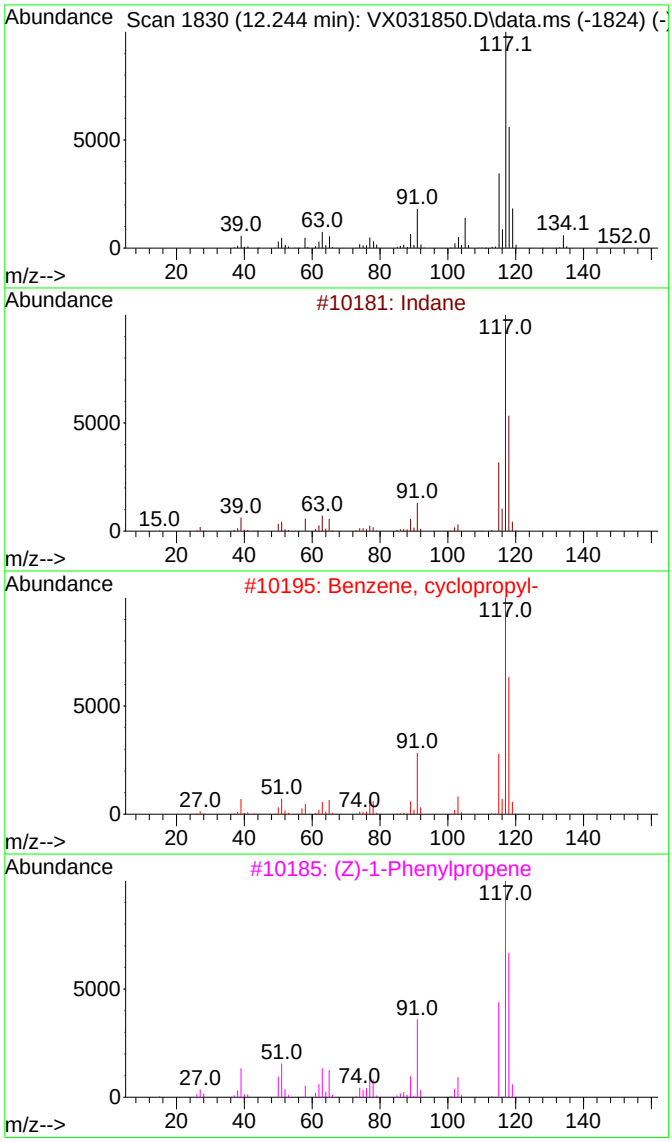
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

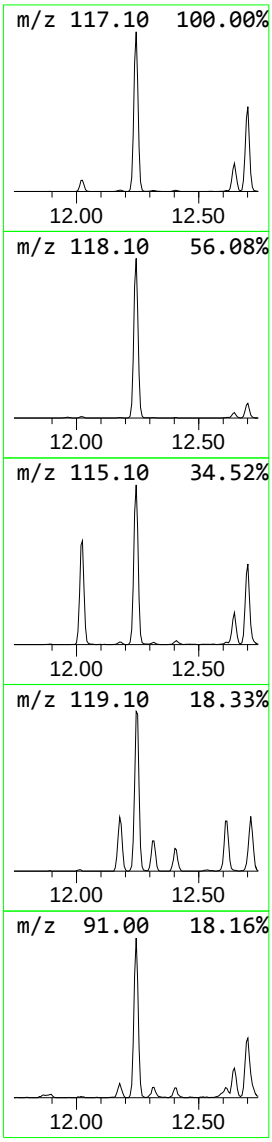
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	77.81 ug/l	638690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	68





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ClientSampleId :
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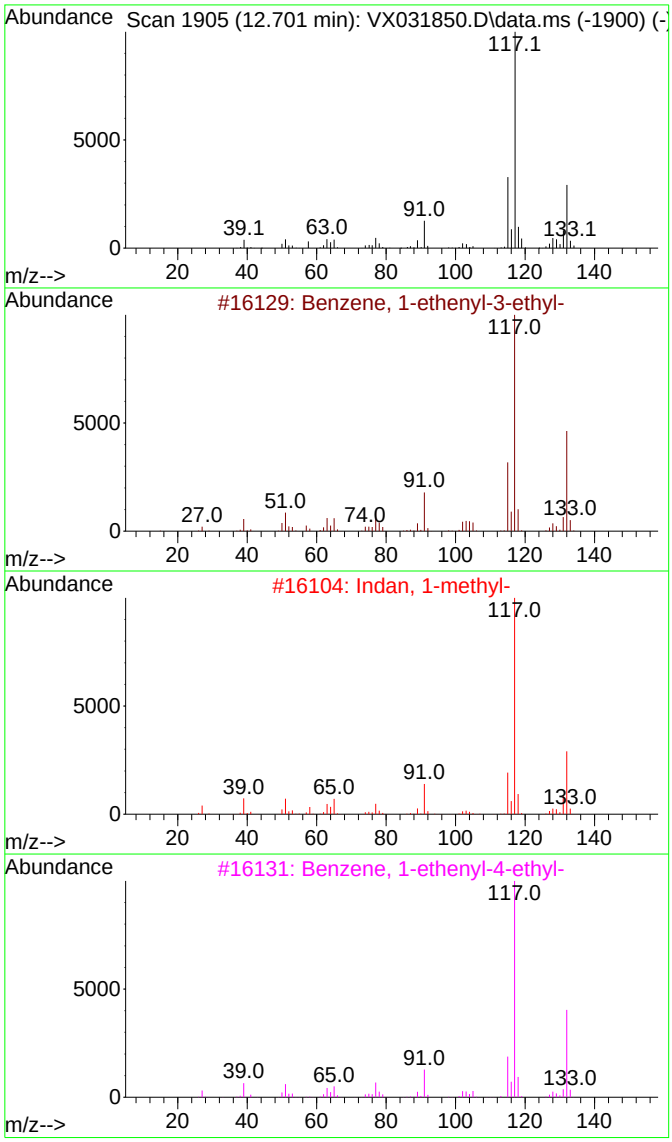
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

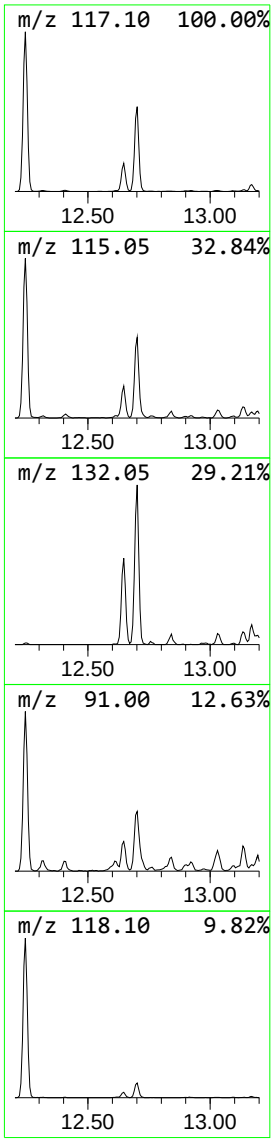
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	36.71 ug/l	301361	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80





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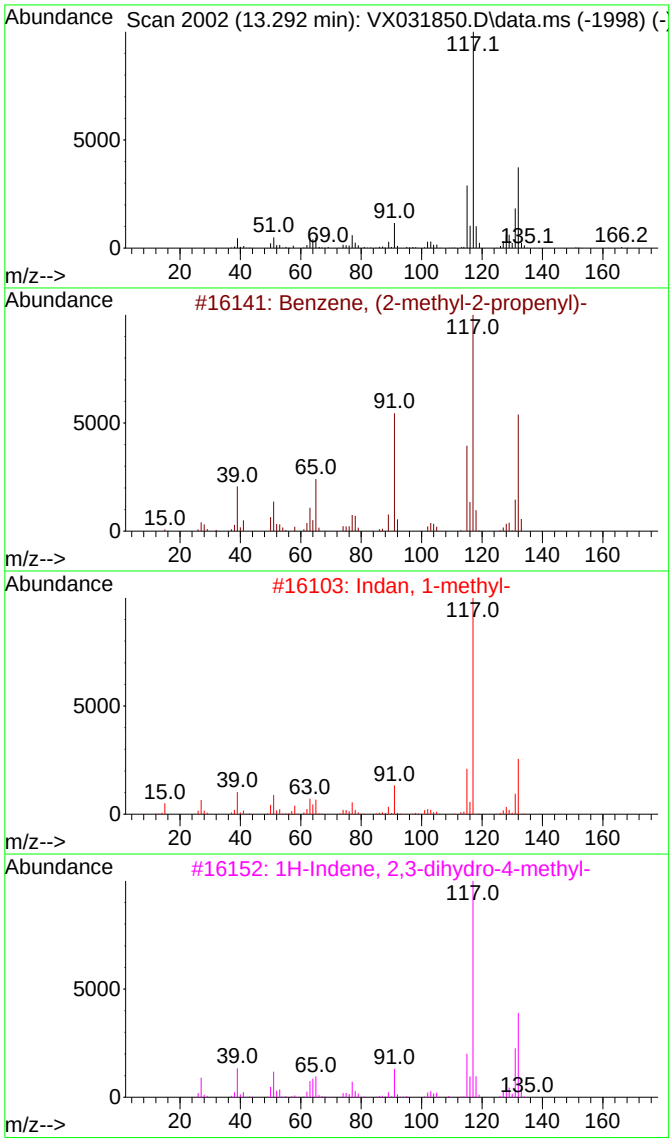
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

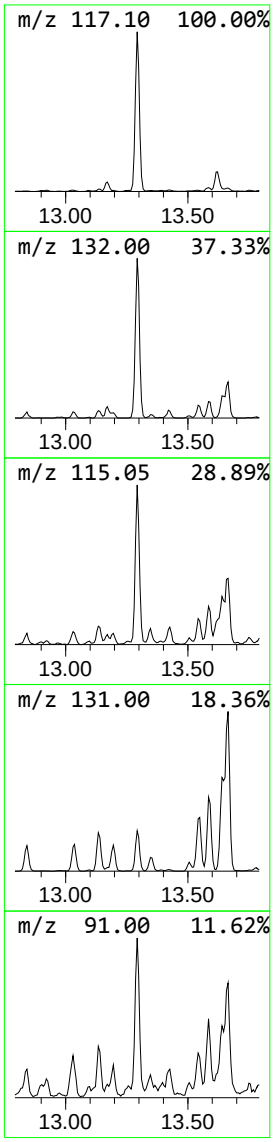
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (2-methyl-2-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	50.22 ug/l	412228	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
2	Indan, 1-methyl-	132	C10H12	000767-58-8	83
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	83
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	81
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	80





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MSVOA_X
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MW-07

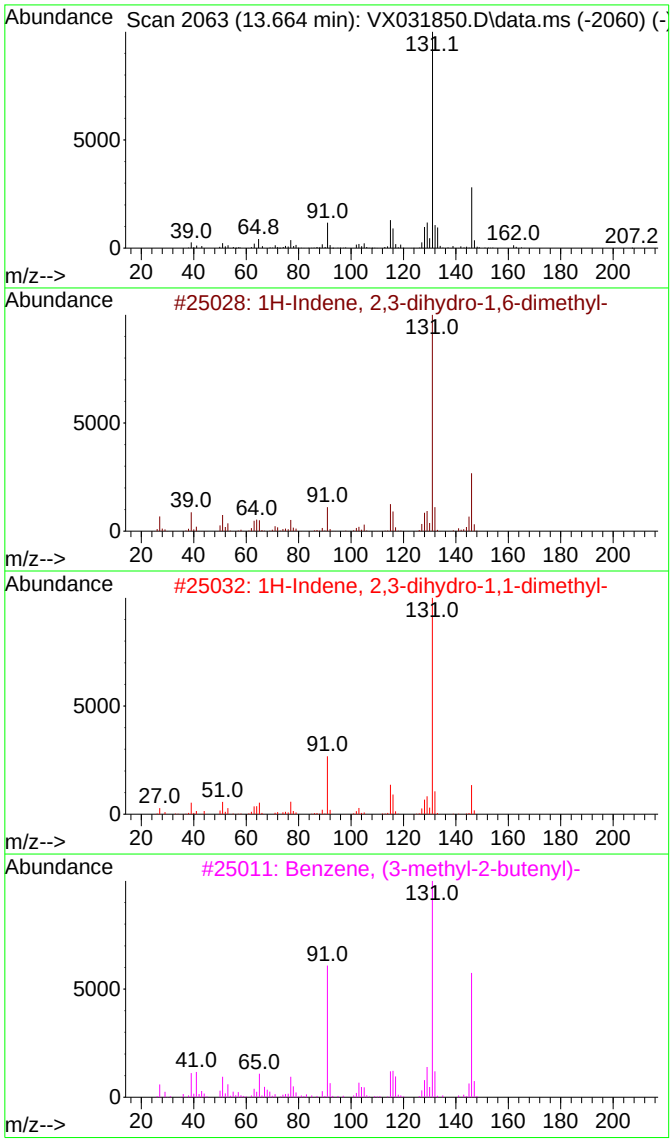
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

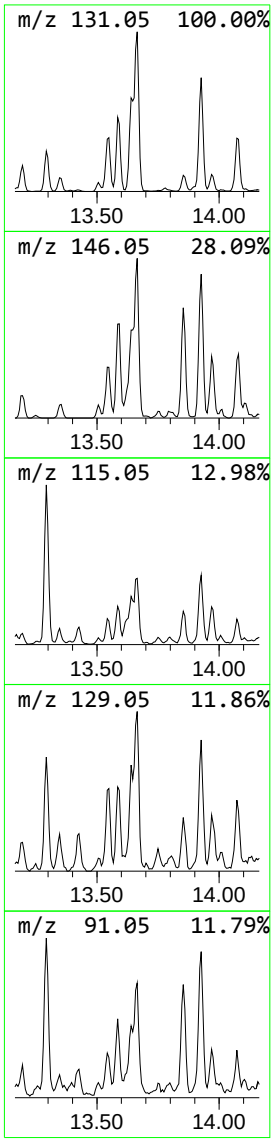
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	34.05 ug/l	279514	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
2	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	91
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	91
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91
5	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	91





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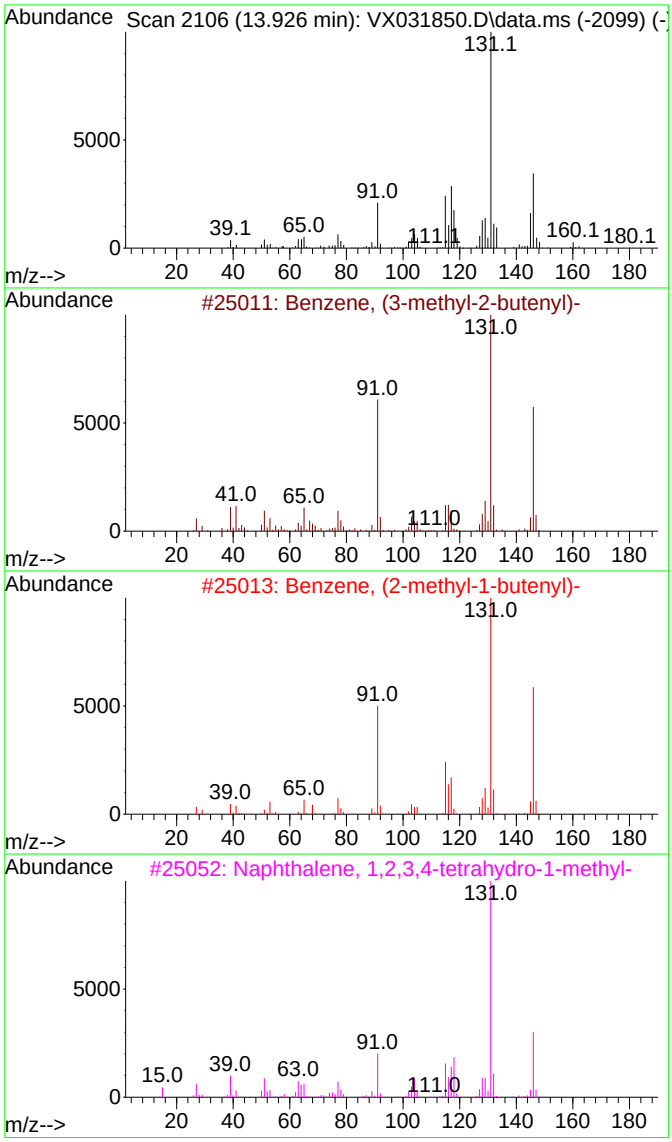
Quant Title : SW846 8260

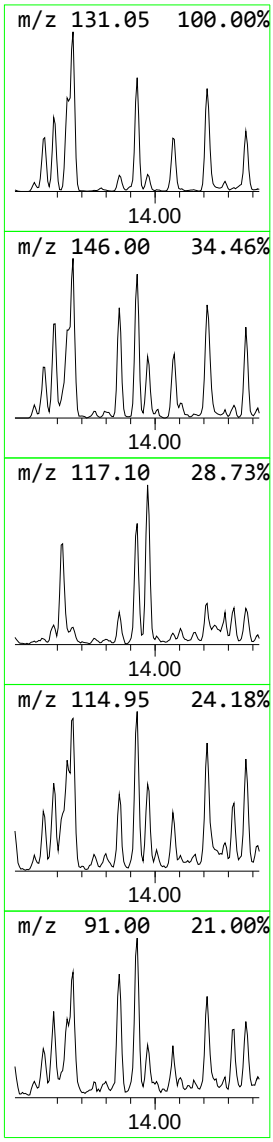
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (3-methyl-2-butenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	36.58 ug/l	300287	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	93
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	89
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	87
4	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	87
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	81





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Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

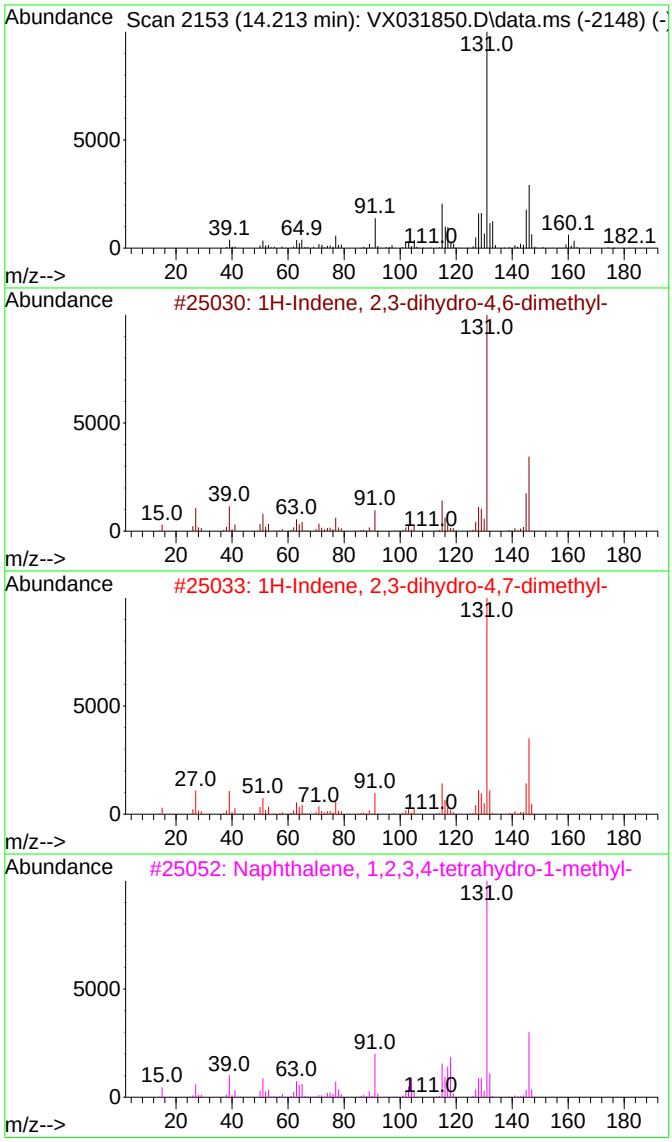
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

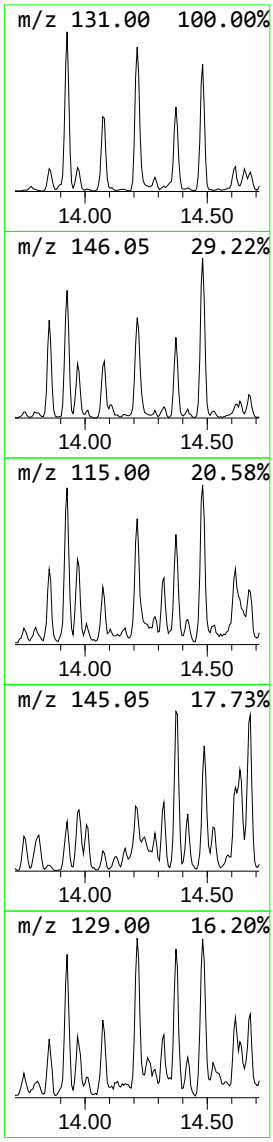
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-4,6-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.213	37.85 ug/l	310687	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	94
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	93
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	87
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

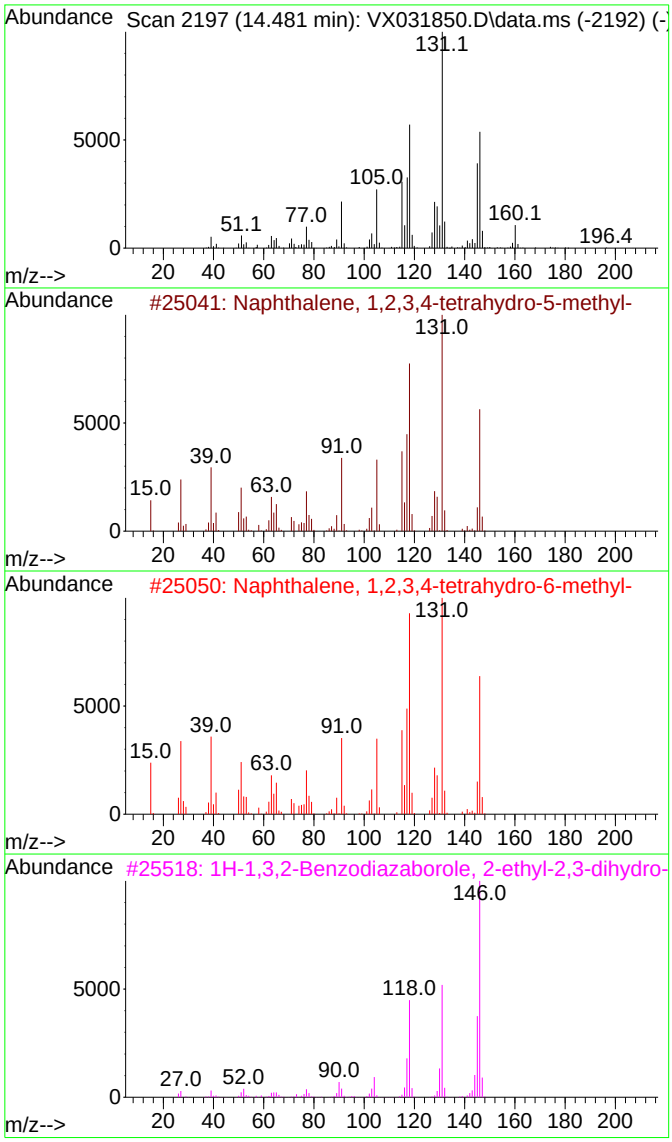
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

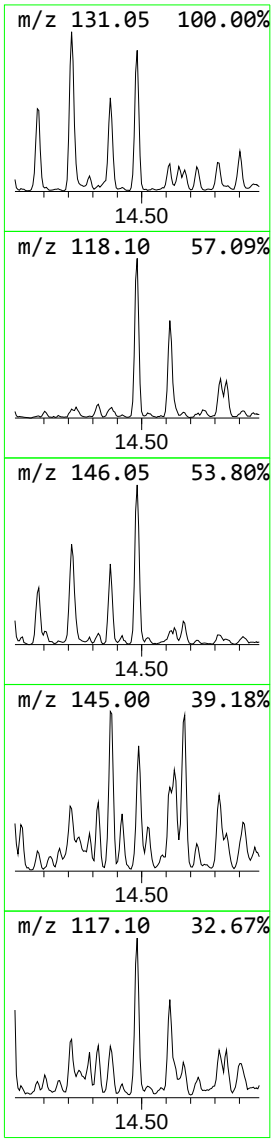
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	44.61 ug/l	366182	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	86
3	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	62
4	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	58
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

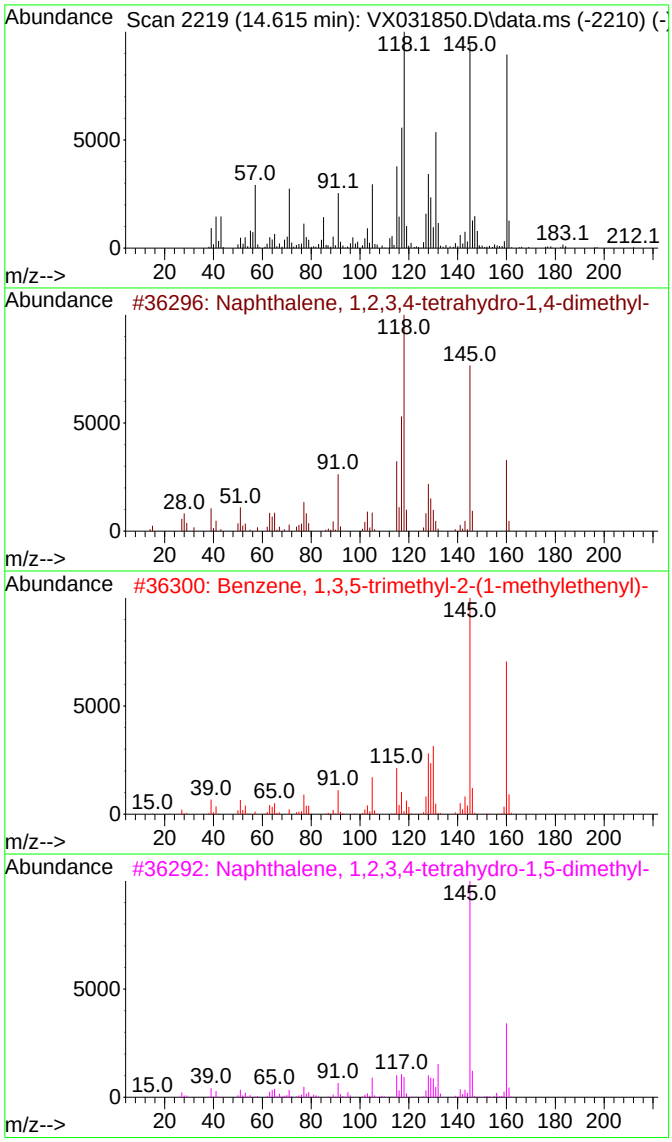
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

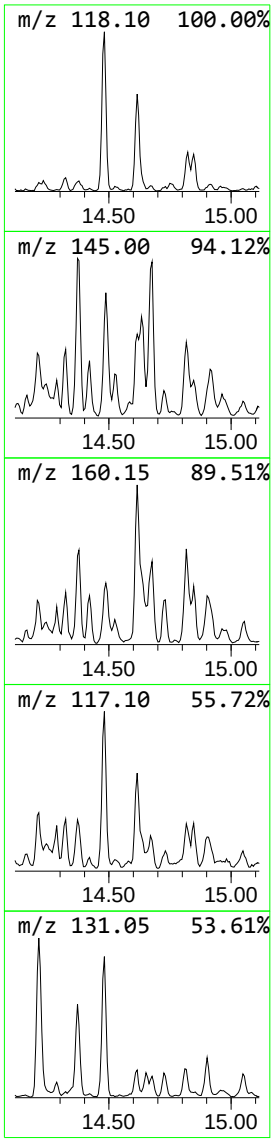
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	39.37 ug/l	323188	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	78
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	76
4	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	60
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

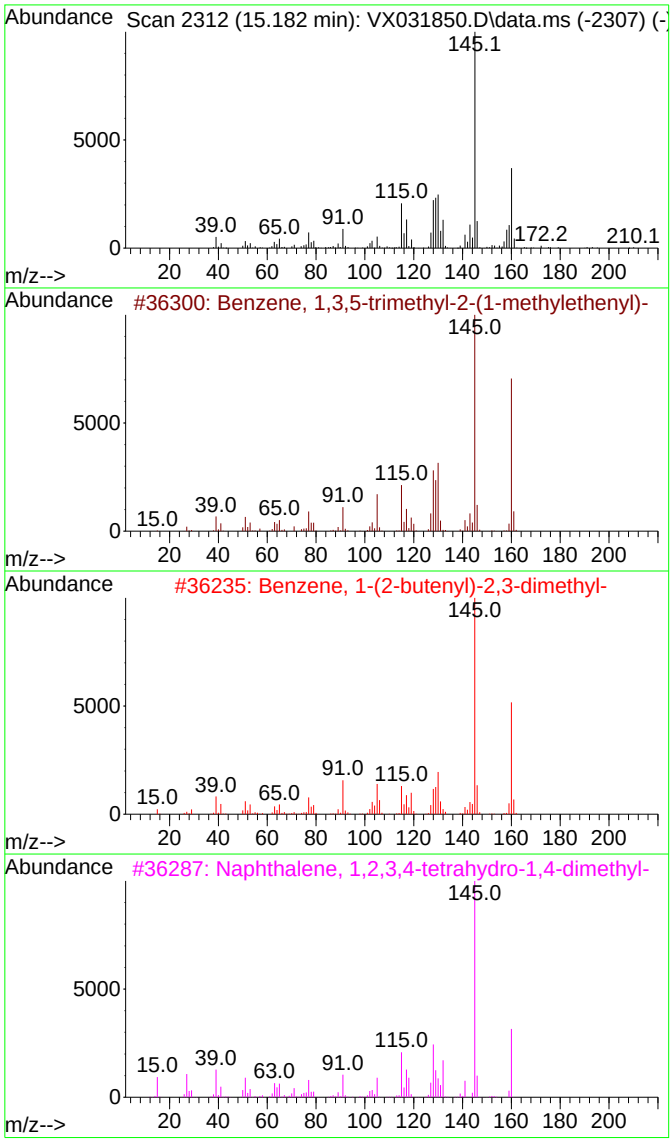
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

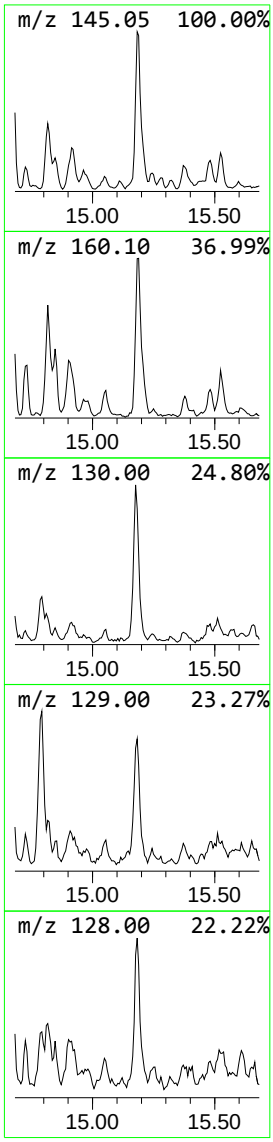
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	28.47 ug/l	233708	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	95
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	81
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	76
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	70
5	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
Data File : VX031850.D
Acq On : 03 Oct 2022 21:44
Operator : JC/MD
Sample : N4860-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-07

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.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
Sulfur dioxide	1.288	74.4	ug/l	324413	1	5.550	218057	50.0
Indane	12.244	77.8	ug/l	638690	4	12.024	410438	50.0
Benzene, 1-ethe...	12.701	36.7	ug/l	301361	4	12.024	410438	50.0
Benzene, (2-met...	13.292	50.2	ug/l	412228	4	12.024	410438	50.0
1H-Indene, 2,3-...	13.664	34.0	ug/l	279514	4	12.024	410438	50.0
Benzene, (3-met...	13.926	36.6	ug/l	300287	4	12.024	410438	50.0
1H-Indene, 2,3-...	14.213	37.9	ug/l	310687	4	12.024	410438	50.0
Naphthalene, 1,...	14.481	44.6	ug/l	366182	4	12.024	410438	50.0
Naphthalene, 1,...	14.615	39.4	ug/l	323188	4	12.024	410438	50.0
Benzene, 1,3,5-...	15.182	28.5	ug/l	233708	4	12.024	410438	50.0