LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
Operator : JC/SP
Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

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\82X012521W.M
Title : SW846 8260

Signal : TIC: VX020781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	60	64	72	rVB	74361	85629	1.86%	0.208%
2	2.331	199	204	213	rVB	33551	66764	1.45%	0.162%
3	5.471	705	719	731	rBV	244996	693241	15.09%	1.681%
4	5.635	734	746	763	rVB	415939	1128709	24.57%	2.738%
5	6.037	800	812	823	rBV	241961	629164	13.70%	1.526%
6	6.836	930	943	958	rBV	622159	1487938	32.39%	3.609%
7	8.696	1242	1248	1255	rVV	1305910	1988977	43.29%	4.824%
8	9.561	1383	1390	1394	rBV4	32270	54736	1.19%	0.133%
9	10.098	1472	1478	1484	rBV	1227362	1677581	36.52%	4.069%
10	10.232	1494	1500	1505	rBV	44991	67643	1.47%	0.164%
11	10.342	1510	1518	1524	rVV	207167	343524	7.48%	0.833%
12	10.396	1524	1527	1540	rVB2	33176	54983	1.20%	0.133%
13	10.622	1557	1564	1568	rBV2	41657	78702	1.71%	0.191%
14	10.683	1568	1574	1583	rVB	128978	193740	4.22%	0.470%
15	10.793	1587	1592	1595	rBV	32779	50653	1.10%	0.123%
16	10.896	1604	1609	1613	rBV2	83077	124206	2.70%	0.301%
17	10.982	1619	1623	1628	rBV2	52102	90170	1.96%	0.219%
18	11.030	1628	1631	1640	rVB2	26803	57871	1.26%	0.140%
19	11.122	1640	1646	1651	rBV	1045884	1300630	28.31%	3.155%
20	11.341	1678	1682	1685	rBV	38760	48628	1.06%	0.118%
21	11.421	1690	1695	1701	rVV	191168	382295	8.32%	0.927%
22	11.488	1701	1706	1708	rVV2	122628	204417	4.45%	0.496%
23	11.518	1708	1711	1715	rVB2	102616	131391	2.86%	0.319%
24	11.652	1728	1733	1739	rBV3	137736	209279	4.56%	0.508%
25	11.793	1751	1756	1761	rBV	478356	613270	13.35%	1.487%
26	11.902	1766	1774	1775	rBV6	41014	85200	1.85%	0.207%
27	11.927	1775	1778	1781	rVV2	42507	65061	1.42%	0.158%
28	11.963	1781	1784	1789	rVV3	102757	186107	4.05%	0.451%
29	12.006	1789	1791	1795	rVV3	73067	87780	1.91%	0.213%
30	12.061	1795	1800	1806	rVB2	1302956	1725450	37.56%	4.185%
31	12.140	1806	1813	1823	rBV2	3394117	4594018	100.00%	11.143%
32	12.286	1833	1837	1838	rBV	107966	133253	2.90%	0.323%
33	12.305	1838	1840	1844	rVB	148518	164900	3.59%	0.400%
34	12.353	1844	1848	1855	rBV4	311270	496462	10.81%	1.204%
35	12.457	1861	1865	1869	rBV3	91620	104972	2.28%	0.255%
36	12.500	1869	1872	1878	rVB3	110232	175120	3.81%	0.425%

LSC Area Percent Report

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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

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
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Title : SW846 8260

37	12.567	1878	1883	1885	rBV2	167570	231502	5.04%	0.562%
38	12.591	1885	1887	1890	rVV	121077	139020	3.03%	0.337%
39	12.652	1894	1897	1900	rVB	123612	140267	3.05%	0.340%
40	12.701	1900	1905	1908	rBV3	97412	153684	3.35%	0.373%
41	12.756	1908	1914	1919	rBV5	154788	330413	7.19%	0.801%
42	12.798	1919	1921	1924	rVB3	47556	47952	1.04%	0.116%
43	12.853	1925	1930	1933	rBV2	369984	514376	11.20%	1.248%
44	12.890	1933	1936	1939	rVB3	288761	321986	7.01%	0.781%
45	12.933	1939	1943	1944	rBV2	56341	70067	1.53%	0.170%
46	12.963	1944	1948	1951	rVB	189234	229994	5.01%	0.558%
47	13.006	1951	1955	1962	rBV4	247517	470166	10.23%	1.140%
48	13.079	1963	1967	1969	rBV4	93819	131925	2.87%	0.320%
49	13.103	1969	1971	1973	rVV	157608	173442	3.78%	0.421%
50	13.134	1973	1976	1981	rVB	454901	551181	12.00%	1.337%
51	13.292	1997	2002	2005	rBV5	101108	201315	4.38%	0.488%
52	13.329	2005	2008	2013	rVB3	511914	680047	14.80%	1.649%
53	13.457	2023	2029	2036	rBV2	2354607	3322143	72.31%	8.058%
54	13.548	2040	2044	2053	rVV5	520417	918003	19.98%	2.227%
55	13.628	2053	2057	2060	rVV3	154710	221838	4.83%	0.538%
56	13.701	2067	2069	2071	rBV	121323	142029	3.09%	0.344%
57	13.743	2073	2076	2080	rVV	667258	810313	17.64%	1.965%
58	13.786	2080	2083	2085	rVV3	194674	289495	6.30%	0.702%
59	13.841	2089	2092	2095	rVB2	221638	260352	5.67%	0.631%
60	13.890	2095	2100	2104	rBV	562472	887885	19.33%	2.154%
61	13.926	2104	2106	2108	rVV2	179517	212816	4.63%	0.516%
62	13.963	2109	2112	2117	rVB4	277213	384734	8.37%	0.933%
63	14.109	2131	2136	2139	rBV5	252543	373703	8.13%	0.906%
64	14.207	2148	2152	2153	rBV3	146901	203474	4.43%	0.494%
65	14.231	2153	2156	2157	rVV3	255971	319489	6.95%	0.775%
66	14.268	2157	2162	2166	rVB3	688090	1111746	24.20%	2.697%
67	14.445	2187	2191	2194	rBV	649407	743951	16.19%	1.804%
68	14.518	2200	2203	2208	rBV2	483074	706239	15.37%	1.713%
69	14.591	2212	2215	2217	rBV3	111902	143397	3.12%	0.348%
70	14.652	2222	2225	2231	rBV	605767	972564	21.17%	2.359%
71	14.713	2231	2235	2239	rVV2	477998	557633	12.14%	1.353%
72	14.792	2245	2248	2251	rBV3	185431	225352	4.91%	0.547%
73	14.829	2251	2254	2257	rVV4	190199	272673	5.94%	0.661%
74	14.883	2261	2263	2268	rVB3	266796	329049	7.16%	0.798%
75	14.999	2280	2282	2291	rVB3	288823	502442	10.94%	1.219%
76	15.225	2315	2319	2322	rBV3	248889	394168	8.58%	0.956%

LSC Area Percent Report

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Instrument : MSVOA_X
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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

77	15.426	2349	2352	2355	rBV2	194985	213778	4.65%	0.519%
78	15.463	2355	2358	2362	rVB	176633	233622	5.09%	0.567%
79	15.609	2377	2382	2387	rVB	1626264	2280679	49.64%	5.532%
80	16.145	2467	2470	2476	rVB7	74685	122836	2.67%	0.298%
81	16.773	2569	2573	2575	rBV3	65924	102135	2.22%	0.248%

Sum of corrected areas: 41228339

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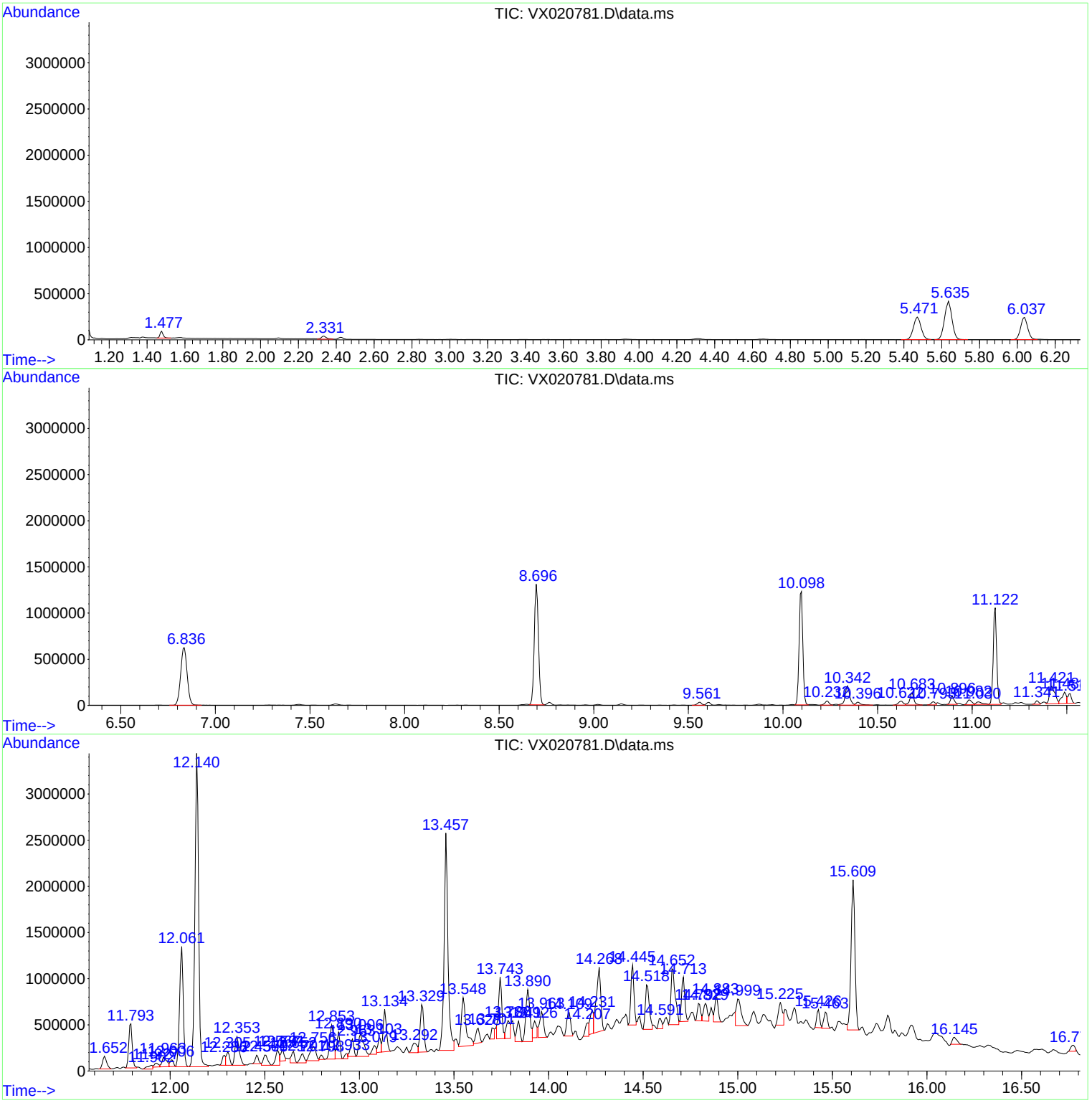
Instrument :
MSVOA_X
ClientSampleId :
1710

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

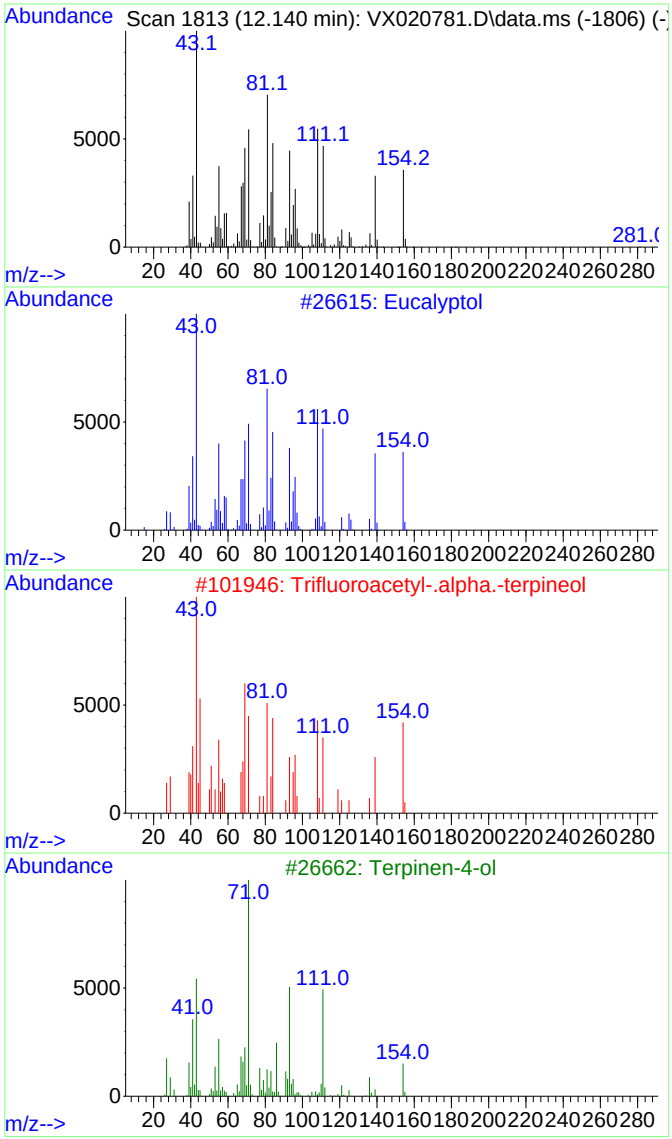
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

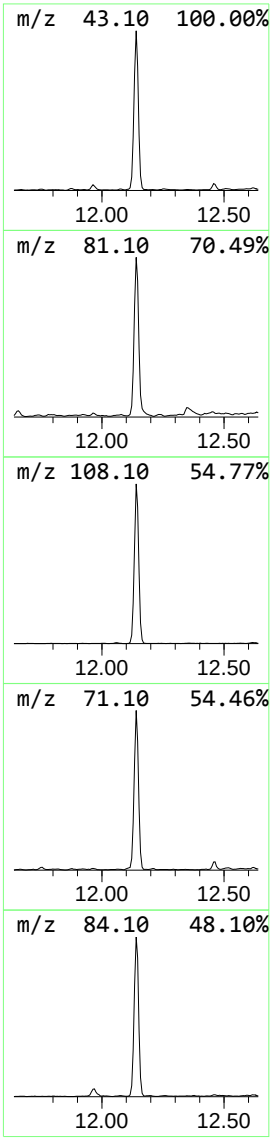
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.140	133.13 ug/l	4594020	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	50
3	Terpinen-4-ol	154	C10H18O	000562-74-3	38
4	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	35
5	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27





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Acq On : 27 Jan 2021 19:31
Operator : JC/SP
Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1710

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

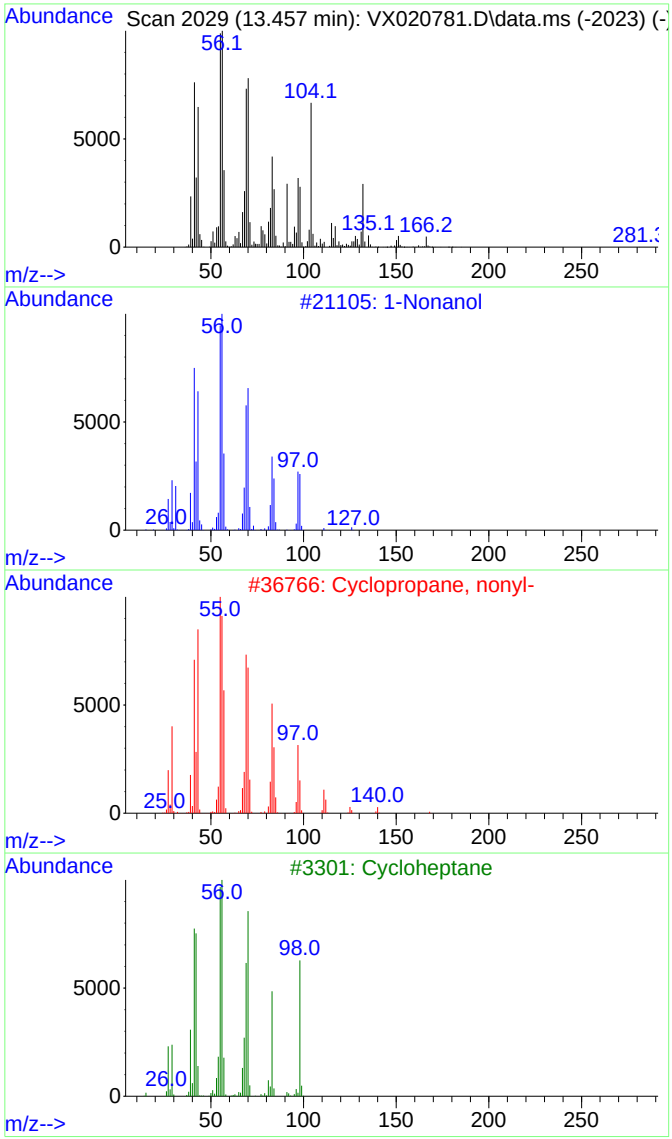
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

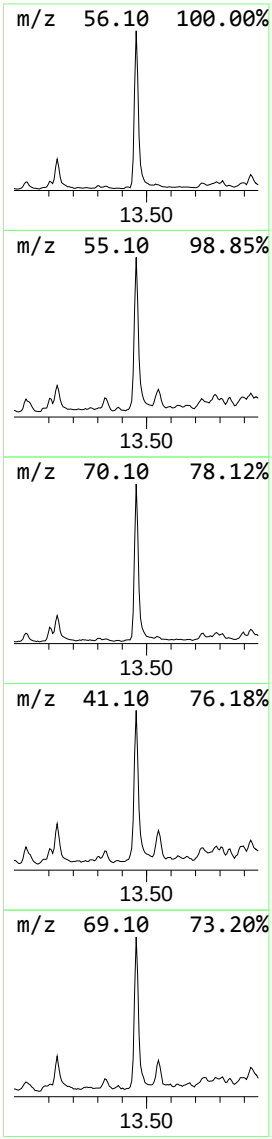
****

Peak Number 2 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	96.27 ug/l	3322140	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	74
2	Cyclopropane, nonyl-	168	C12H24	074663-85-7	72
3	Cycloheptane	98	C7H14	000291-64-5	62
4	3-Heptene	98	C7H14	000592-78-9	43
5	(Z)-3-Heptene	98	C7H14	007642-10-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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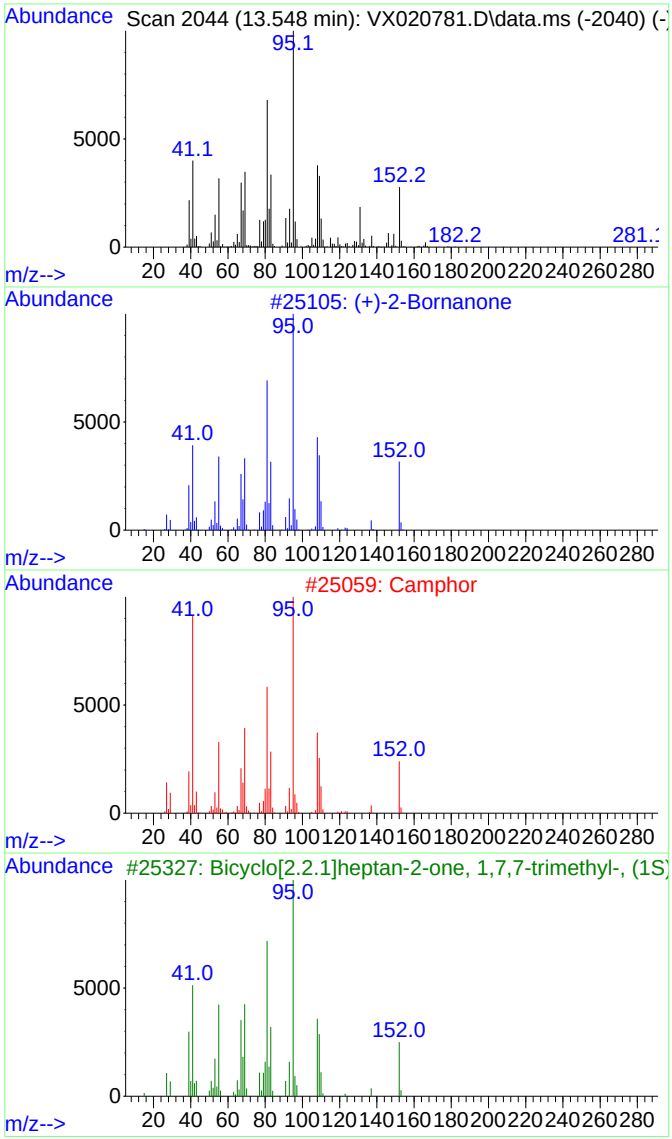
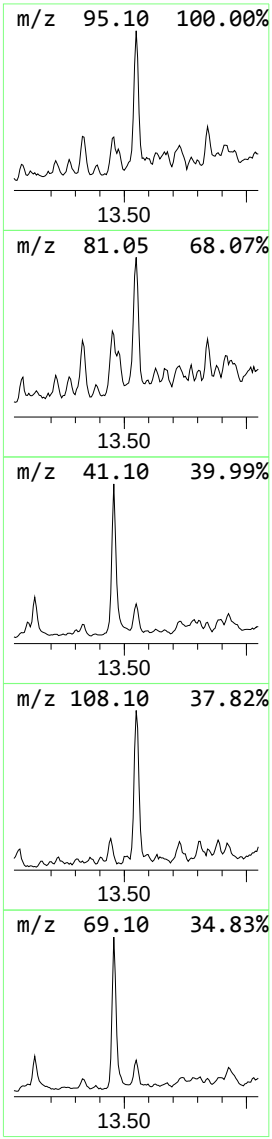
****

Peak Number 3 (+)-2-Bornanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.548	26.60 ug/l	918003	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2	Camphor	152	C10H16O	000076-22-2	94
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	93
4	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	46
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





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Instrument : MSVOA_X
ClientSampleId : 1710

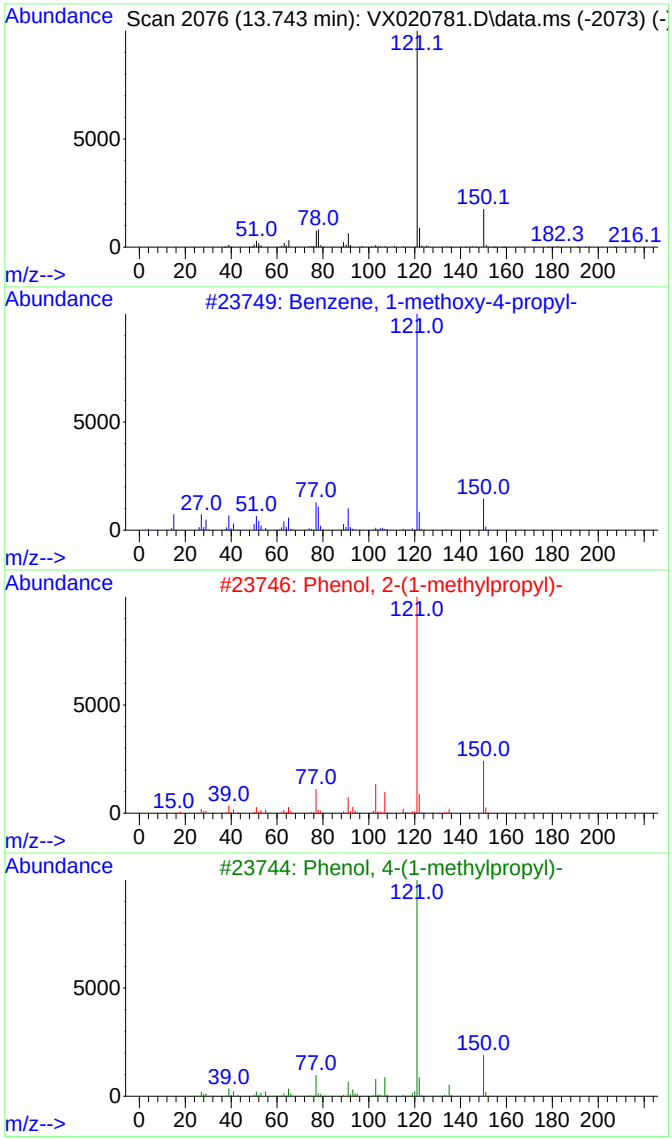
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

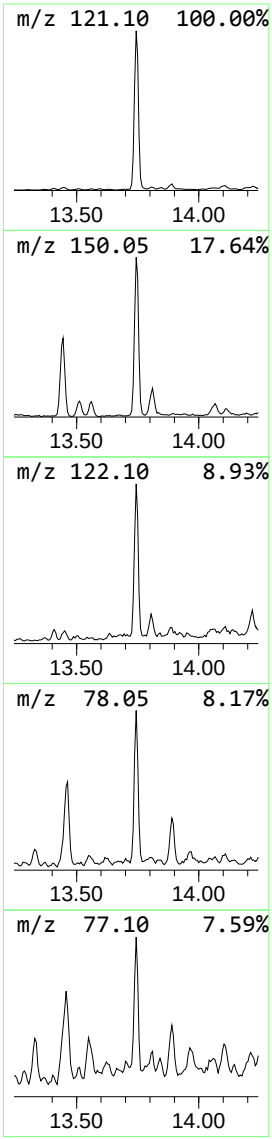
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-methoxy-4-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.743	23.48 ug/l	810313	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	78
3	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	72
4	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	72
5	4-(4-Methoxyphenyl)-1-butanol	180	C11H16O2	052244-70-9	72





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1710

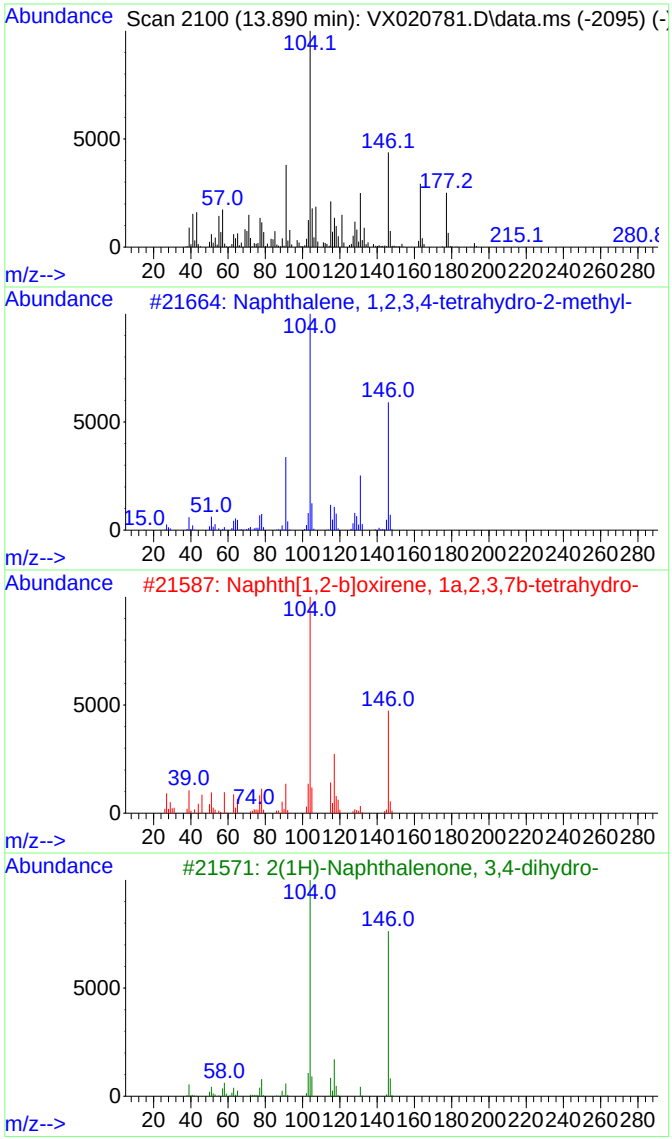
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

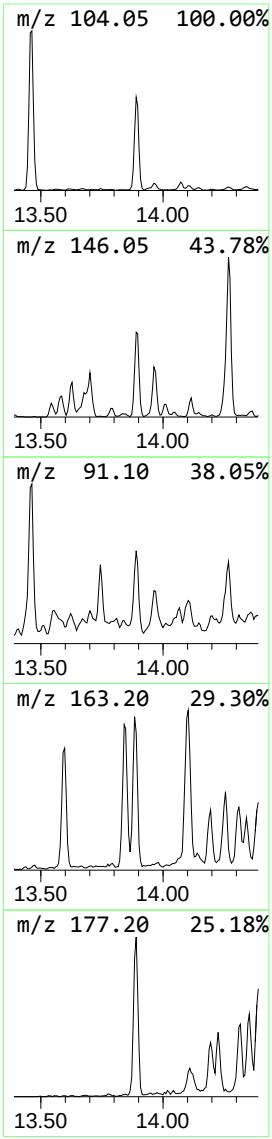
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.890	25.73 ug/l	887885	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	91
2	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	49
3	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	49
4	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	38
5	2,6-Piperidinedione, 3-phenyl-	189	C11H11NO2	014149-34-9	35





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Instrument : MSVOA_X
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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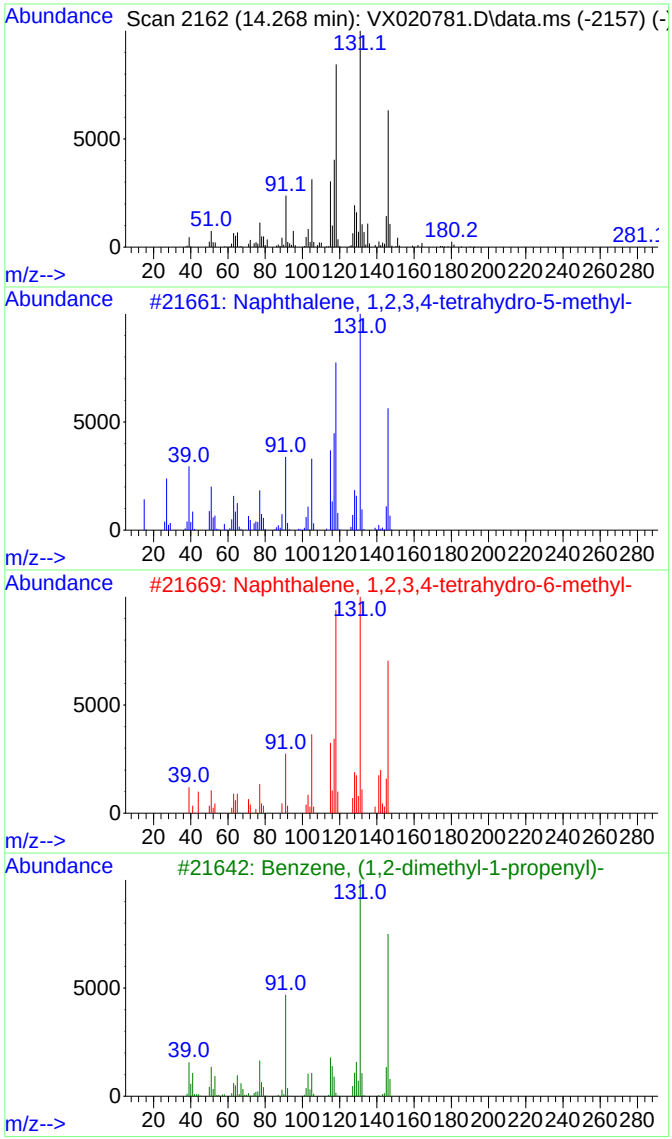
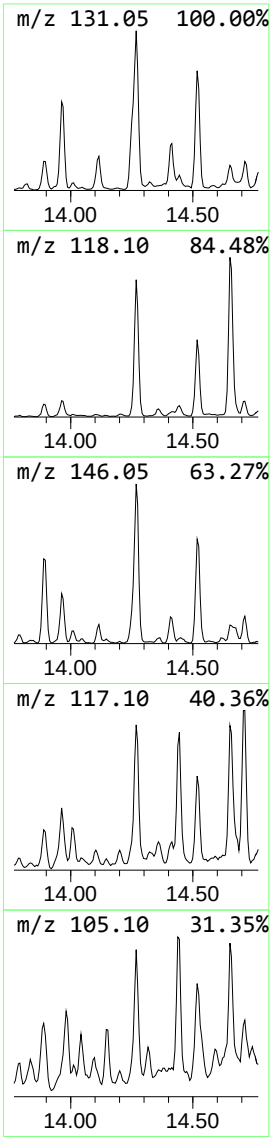
****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	32.22 ug/l	1111750	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	55
5	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
Operator : JC/SP
Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

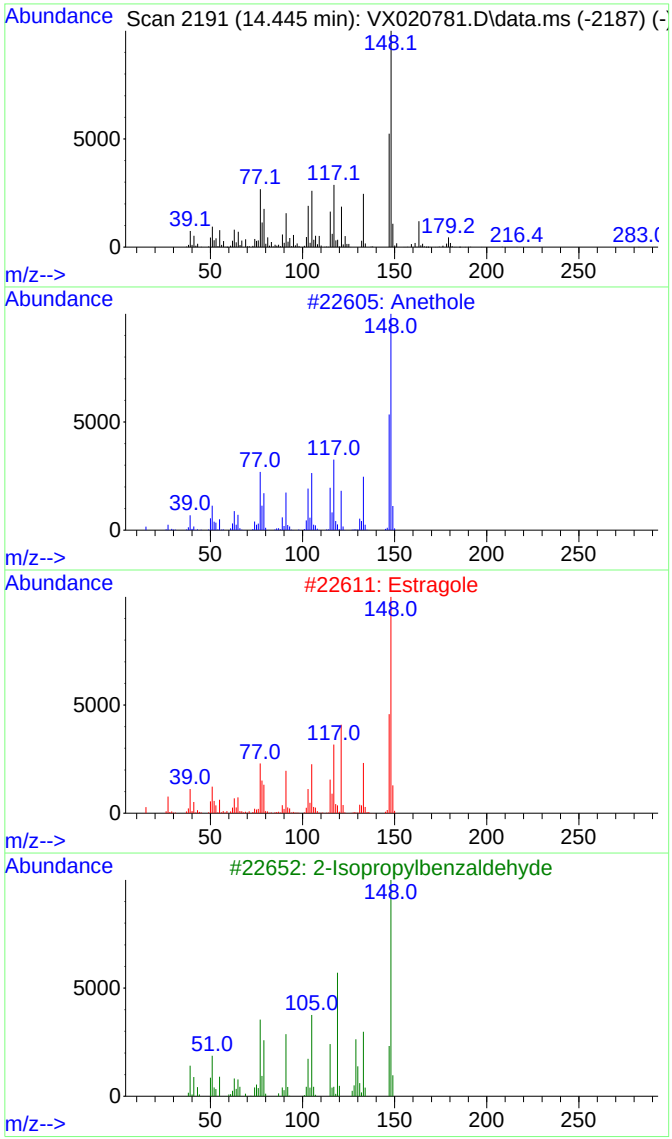
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

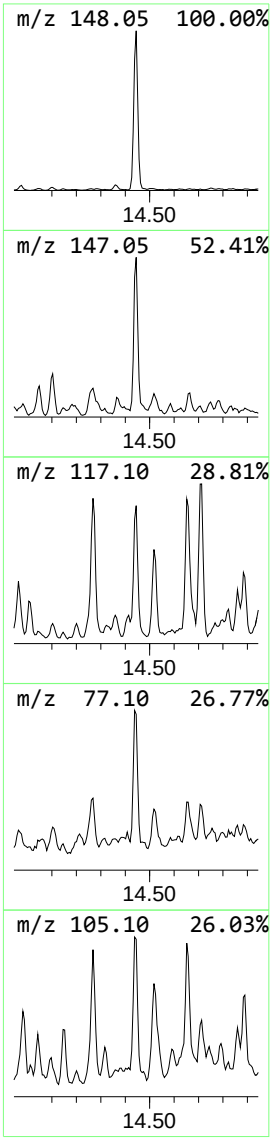
****

Peak Number 7 Anethole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	21.56 ug/l	743951	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole	148	C10H12O	000104-46-1	95
2	Estragole	148	C10H12O	000140-67-0	80
3	2-Isopropylbenzaldehyde	148	C10H12O	006502-22-3	52
4	N-Amino-1,2,3,4-tetrahydroquinoline	148	C9H12N2	1000305-92-6	50
5	Methanimidamide, N,N-dimethyl-N'...	148	C9H12N2	001783-25-1	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
Operator : JC/SP
Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1710

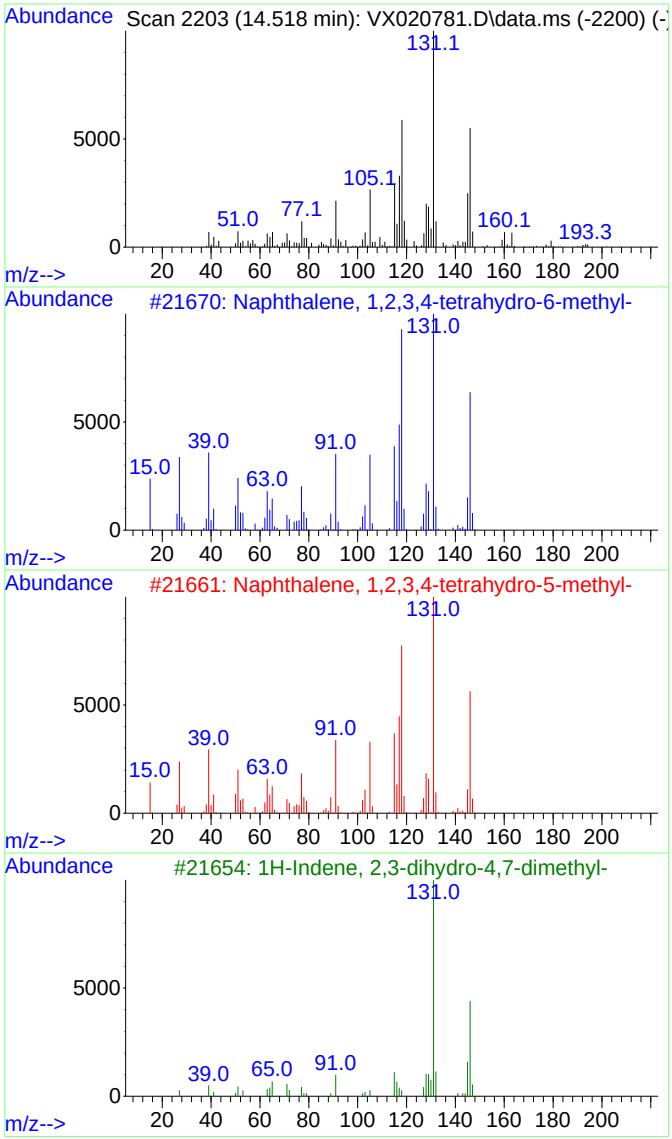
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

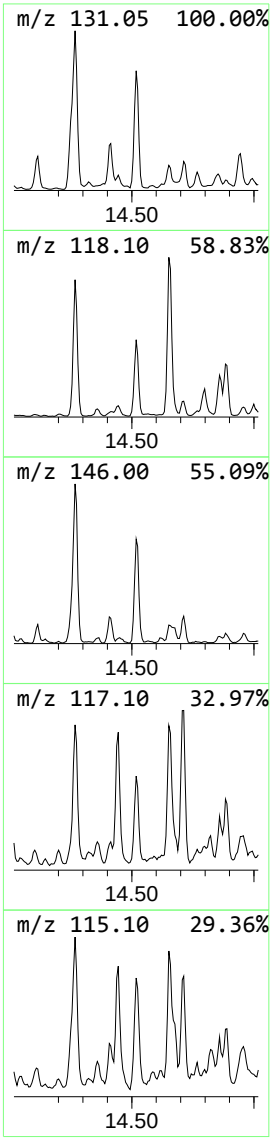
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.518	20.47 ug/l	706239	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
Operator : JC/SP
Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

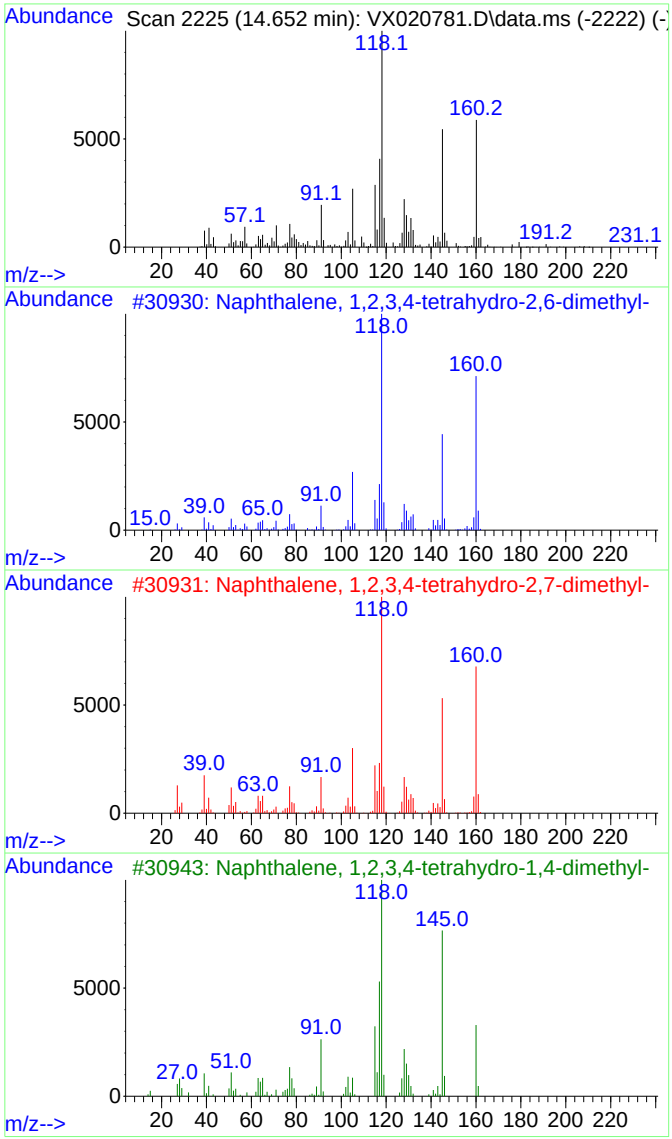
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

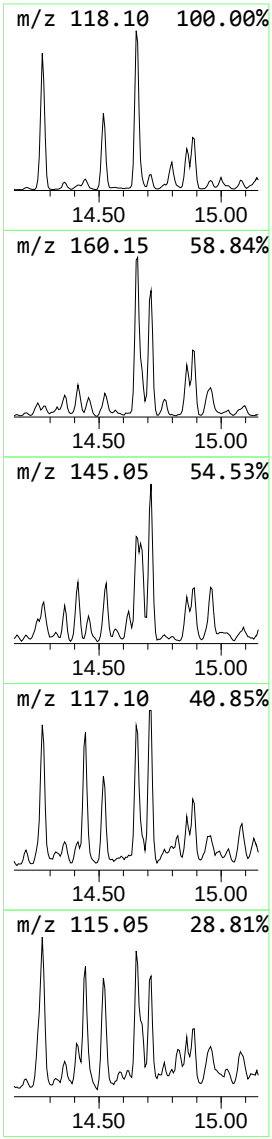
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.652	28.18 ug/l	972564	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	81
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	81
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	74
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	58
5	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	52





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Sample : M1217-16 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1710

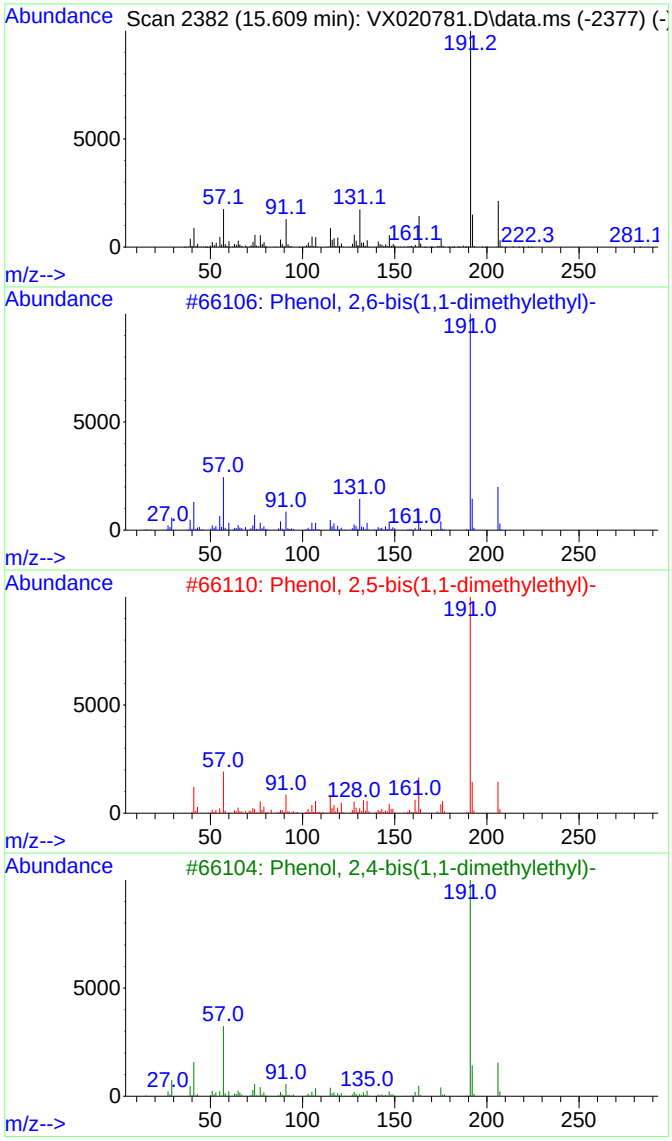
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

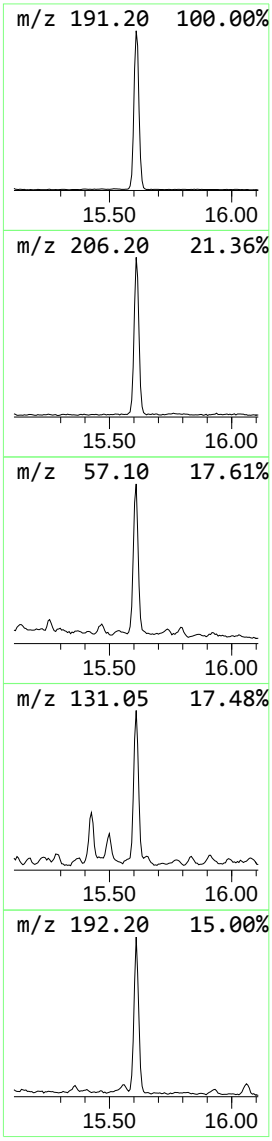
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	66.09 ug/l	2280680	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
3	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	83
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
5	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
Data File : VX020781.D
Acq On : 27 Jan 2021 19:31
Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1710

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Eucalyptol	12.140	133.1	ug/l	4594020	4	12.061	1725450	50.0
1-Nonanol	13.457	96.3	ug/l	3322140	4	12.061	1725450	50.0
(+)-2-Bornanone	13.548	26.6	ug/l	918003	4	12.061	1725450	50.0
Benzene, 1-meth...	13.743	23.5	ug/l	810313	4	12.061	1725450	50.0
Naphthalene, 1,...	13.890	25.7	ug/l	887885	4	12.061	1725450	50.0
Naphthalene, 1,...	14.268	32.2	ug/l	1111750	4	12.061	1725450	50.0
Anethole	14.445	21.6	ug/l	743951	4	12.061	1725450	50.0
Naphthalene, 1,...	14.518	20.5	ug/l	706239	4	12.061	1725450	50.0
Naphthalene, 1,...	14.652	28.2	ug/l	972564	4	12.061	1725450	50.0
Phenol, 2,6-bis...	15.609	66.1	ug/l	2280680	4	12.061	1725450	50.0