LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122923\
Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
Sample : 06017-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

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\82X121323W.M
Title : SW846 8260

Signal : TIC: VX039538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	689	706	714	rBV	58272	185570	12.67%	0.640%
2	5.483	714	721	725	rVV2	43295	124623	8.51%	0.430%
3	5.544	725	731	757	rVB2	100632	388138	26.50%	1.339%
4	5.806	762	774	787	rBV2	53205	154356	10.54%	0.533%
5	5.958	789	799	807	rBV2	71979	209089	14.27%	0.722%
6	6.233	834	844	855	rVV	127331	396414	27.06%	1.368%
7	6.599	895	904	913	rBV2	48855	117557	8.03%	0.406%
8	6.757	921	930	940	rBV	180837	466198	31.83%	1.609%
9	7.367	1019	1030	1042	rVB4	41347	114888	7.84%	0.396%
10	7.489	1042	1050	1055	rBV	51499	106537	7.27%	0.368%
11	7.550	1055	1060	1072	rVV	67068	159791	10.91%	0.551%
12	7.976	1120	1130	1142	rVB	144190	314490	21.47%	1.085%
13	8.098	1142	1150	1158	rBV2	121994	272966	18.64%	0.942%
14	8.184	1158	1164	1169	rVV	78996	144612	9.87%	0.499%
15	8.269	1173	1178	1182	rBV	170709	288953	19.73%	0.997%
16	8.306	1182	1184	1190	rVB	83420	117566	8.03%	0.406%
17	8.434	1200	1205	1214	rBV	186194	334934	22.87%	1.156%
18	8.610	1226	1234	1236	rBV3	108709	223373	15.25%	0.771%
19	8.647	1236	1240	1248	rVB	386205	637664	43.53%	2.200%
20	8.909	1277	1283	1290	rBV2	134903	232743	15.89%	0.803%
21	9.098	1306	1314	1320	rBV3	41343	102459	7.00%	0.354%
22	9.159	1320	1324	1327	rVV2	40322	68643	4.69%	0.237%
23	9.196	1327	1330	1340	rVB4	34677	62715	4.28%	0.216%
24	9.287	1340	1345	1350	rBV	44569	64286	4.39%	0.222%
25	9.385	1355	1361	1366	rBV3	69659	118493	8.09%	0.409%
26	9.494	1374	1379	1386	rBV2	129822	258199	17.63%	0.891%
27	9.647	1402	1404	1415	rVB7	33140	97307	6.64%	0.336%
28	9.756	1416	1422	1428	rBV3	52217	107814	7.36%	0.372%
29	9.817	1428	1432	1436	rBV2	53998	107273	7.32%	0.370%
30	9.866	1437	1440	1442	rVV3	51336	79913	5.46%	0.276%
31	9.903	1442	1446	1451	rVB	412205	573661	39.16%	1.980%
32	10.006	1458	1463	1467	rBV	333042	423500	28.91%	1.461%
33	10.055	1467	1471	1476	rBV	404133	564140	38.51%	1.947%
34	10.195	1489	1494	1499	rVB	118767	171713	11.72%	0.593%
35	10.256	1499	1504	1509	rBV3	65060	160902	10.99%	0.555%
36	10.305	1509	1512	1516	rVB2	66594	104664	7.15%	0.361%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
SB32-2-20231222-7.5-8.5-A

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Title : SW846 8260

37	10.360	1516	1521	1532	rVB5	197660	416771	28.45%	1.438%
38	10.586	1553	1558	1561	rBV	117116	148588	10.14%	0.513%
39	10.671	1567	1572	1577	rBV	99322	161059	11.00%	0.556%
40	10.756	1582	1586	1587	rBV2	51872	70959	4.84%	0.245%
41	10.781	1587	1590	1593	rVB	133131	151563	10.35%	0.523%
42	10.854	1593	1602	1607	rBV2	111451	207317	14.15%	0.715%
43	10.964	1613	1620	1627	rBV2	97178	201192	13.74%	0.694%
44	11.031	1627	1631	1634	rBV2	90294	135424	9.25%	0.467%
45	11.086	1634	1640	1642	rVV2	488883	747786	51.05%	2.580%
46	11.110	1642	1644	1650	rVB2	361671	497859	33.99%	1.718%
47	11.189	1650	1657	1665	rVB	271713	401939	27.44%	1.387%
48	11.305	1672	1676	1683	rVB	344286	423832	28.94%	1.463%
49	11.396	1686	1691	1694	rVB	37355	61864	4.22%	0.213%
50	11.433	1694	1697	1700	rBV	43803	59129	4.04%	0.204%
51	11.476	1700	1704	1711	rVB2	208400	315197	21.52%	1.088%
52	11.628	1723	1729	1734	rBV3	77630	159236	10.87%	0.549%
53	11.683	1734	1738	1740	rBV	66050	78560	5.36%	0.271%
54	11.713	1740	1743	1746	rVB	69659	65112	4.45%	0.225%
55	11.750	1746	1749	1753	rBV2	85291	136093	9.29%	0.470%
56	11.835	1759	1763	1766	rBV	93694	137748	9.40%	0.475%
57	11.866	1766	1768	1770	rVV	52074	53858	3.68%	0.186%
58	11.890	1770	1772	1775	rVB	87747	83810	5.72%	0.289%
59	11.933	1775	1779	1783	rBV2	92149	138893	9.48%	0.479%
60	12.024	1788	1794	1799	rBV2	453777	756714	51.66%	2.611%
61	12.073	1799	1802	1804	rBV	84717	95062	6.49%	0.328%
62	12.098	1804	1806	1809	rVB2	97399	99229	6.77%	0.342%
63	12.171	1816	1818	1825	rVB2	161812	191597	13.08%	0.661%
64	12.244	1825	1830	1836	rBV	827913	1113523	76.02%	3.842%
65	12.311	1836	1841	1844	rBV	336802	518660	35.41%	1.790%
66	12.421	1853	1859	1863	rVV3	114181	201987	13.79%	0.697%
67	12.463	1863	1866	1873	rVB2	143496	216829	14.80%	0.748%
68	12.530	1873	1877	1882	rBV	125462	175363	11.97%	0.605%
69	12.579	1882	1885	1886	rVV	52799	61406	4.19%	0.212%
70	12.610	1886	1890	1894	rVV	1023441	1321040	90.19%	4.559%
71	12.646	1894	1896	1900	rVV	143439	167074	11.41%	0.577%
72	12.701	1900	1905	1914	rVB2	384984	719914	49.15%	2.484%
73	12.799	1916	1921	1926	rVV6	26988	62894	4.29%	0.217%
74	12.921	1933	1941	1945	rBV	679421	983961	67.18%	3.395%
75	12.963	1945	1948	1954	rVB	643751	802918	54.82%	2.771%
76	13.024	1954	1958	1967	rBV3	177568	366535	25.02%	1.265%

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Integrator: RTE
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Title : SW846 8260

77	13.116	1967	1973	1975	rBV2	61645	93854	6.41%	0.324%
78	13.140	1975	1977	1978	rVV2	60817	58864	4.02%	0.203%
79	13.171	1978	1982	1986	rVV	529657	634700	43.33%	2.190%
80	13.213	1986	1989	1992	rVB	92486	100533	6.86%	0.347%
81	13.262	1992	1997	1998	rBV2	131951	177315	12.11%	0.612%
82	13.292	1998	2002	2008	rVV2	1017962	1464739	100.00%	5.054%
83	13.372	2012	2015	2020	rVB	188726	227787	15.55%	0.786%
84	13.420	2020	2023	2032	rVB2	147604	255941	17.47%	0.883%
85	13.506	2032	2037	2040	rBV2	140267	218634	14.93%	0.754%
86	13.542	2040	2043	2046	rVV	246869	313915	21.43%	1.083%
87	13.579	2046	2049	2056	rVV3	321919	561968	38.37%	1.939%
88	13.664	2056	2063	2069	rVB2	208771	435936	29.76%	1.504%
89	13.774	2077	2081	2087	rVB	774216	970224	66.24%	3.348%
90	13.926	2099	2106	2110	rBV2	153663	260348	17.77%	0.898%
91	13.969	2110	2113	2117	rBV	95320	114668	7.83%	0.396%
92	14.073	2126	2130	2134	rBV	221228	279851	19.11%	0.966%
93	14.213	2148	2153	2159	rBV	213255	336461	22.97%	1.161%
94	14.323	2167	2171	2176	rBV	101445	142515	9.73%	0.492%
95	14.372	2176	2179	2183	rVB	134155	157532	10.75%	0.544%
96	14.481	2192	2197	2202	rBV5	35354	75872	5.18%	0.262%
97	14.634	2214	2222	2227	rBV	602825	783288	53.48%	2.703%
98	14.780	2240	2246	2251	rVV	303401	397574	27.14%	1.372%
99	15.475	2355	2360	2372	rVB	44015	79900	5.45%	0.276%
100	15.615	2377	2383	2386	rVV	44669	72153	4.93%	0.249%

Sum of corrected areas: 28979211

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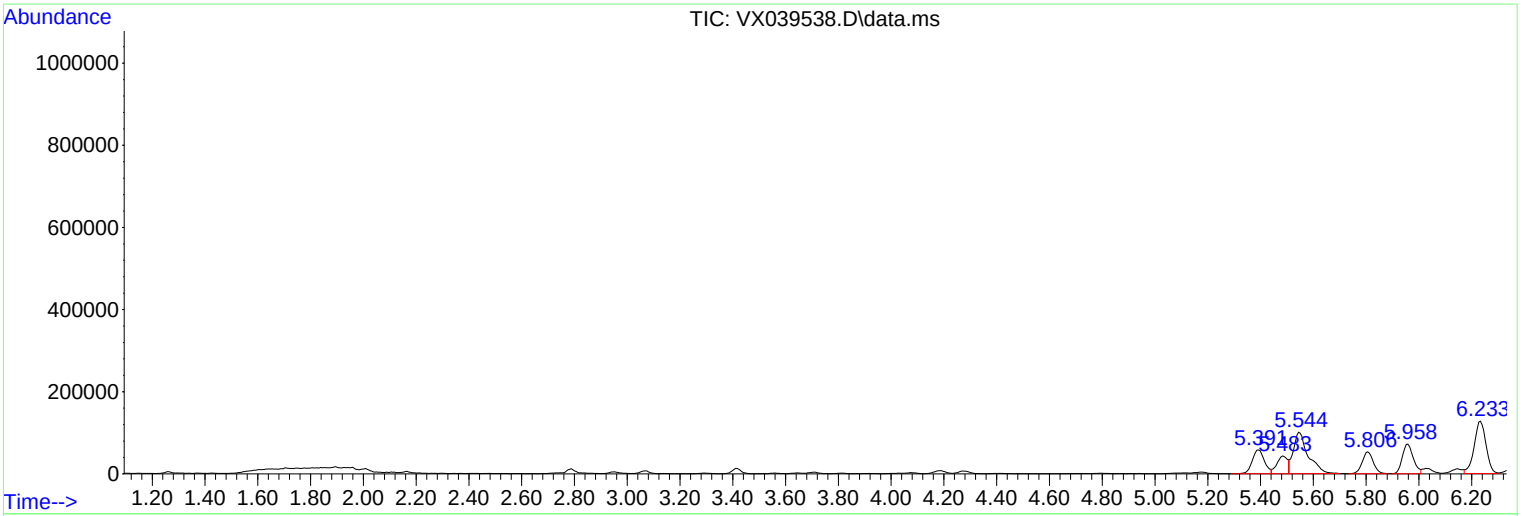
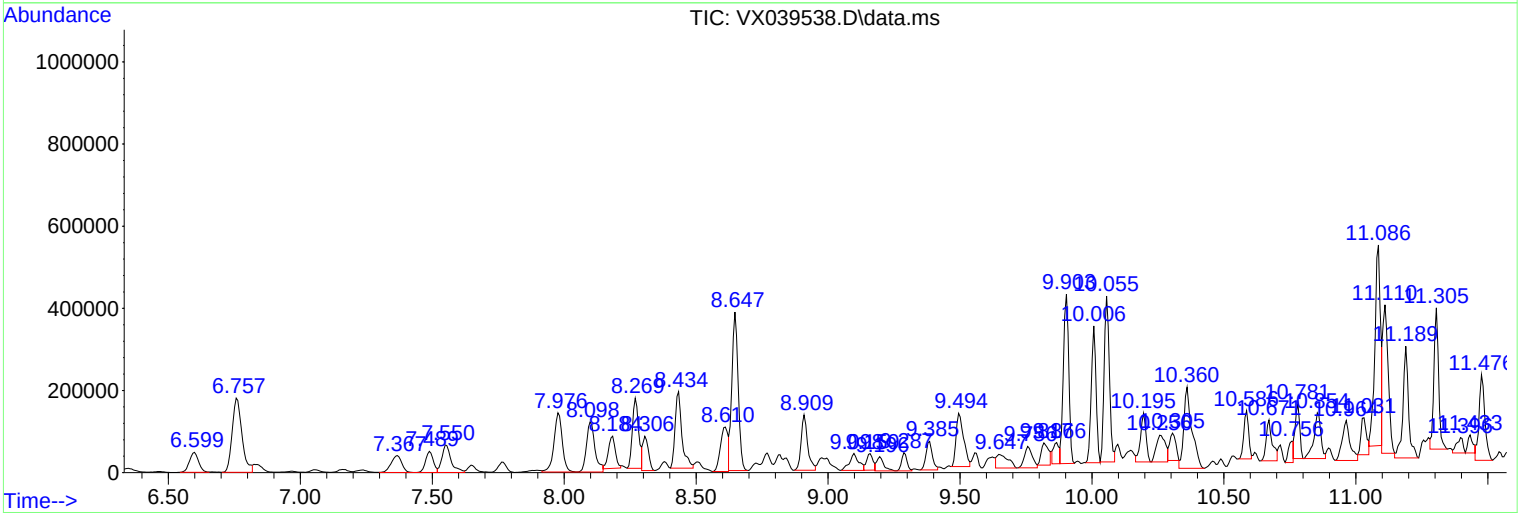
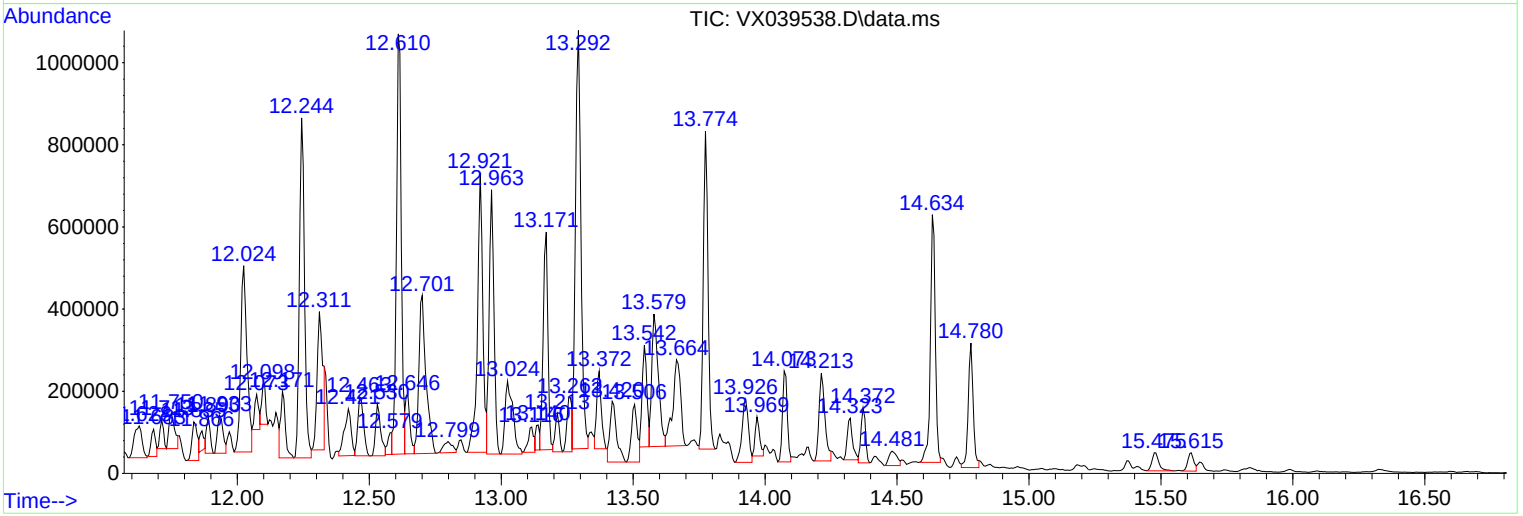
Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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







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MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

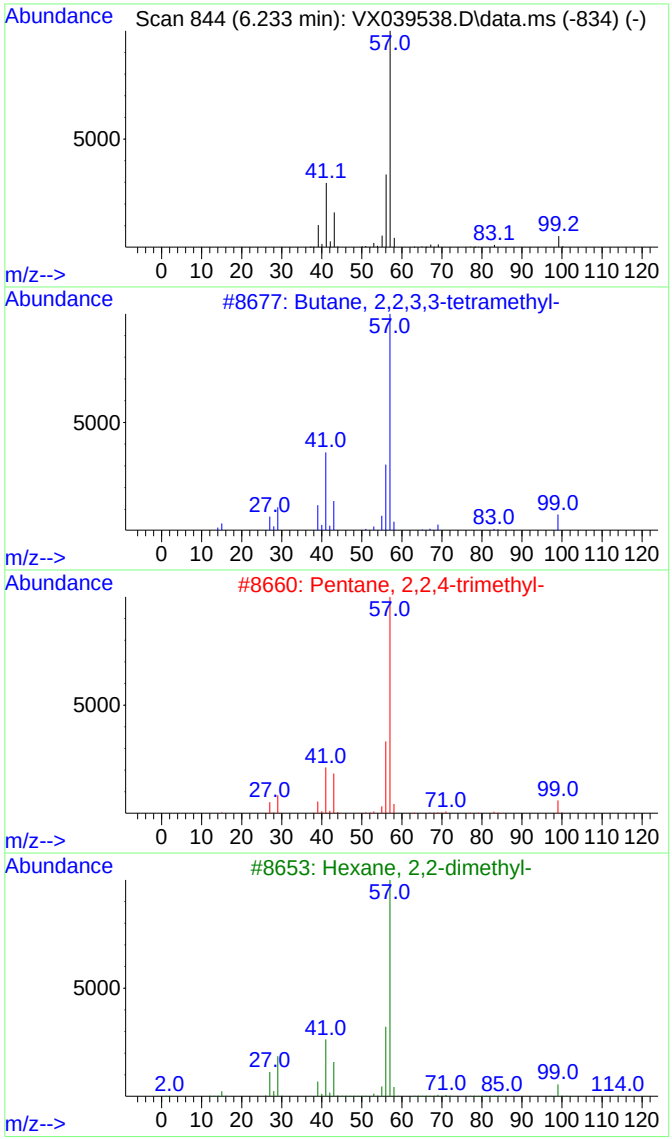
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

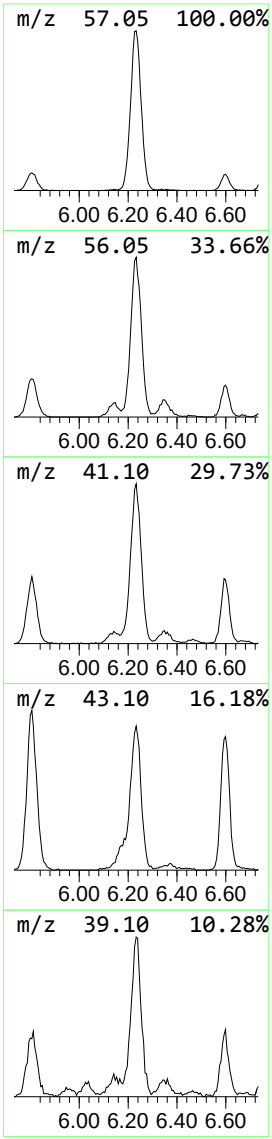
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2,2,3,3-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	42.52 ug/l	396414	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59





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SB32-2-20231222-7.5-8.5-A

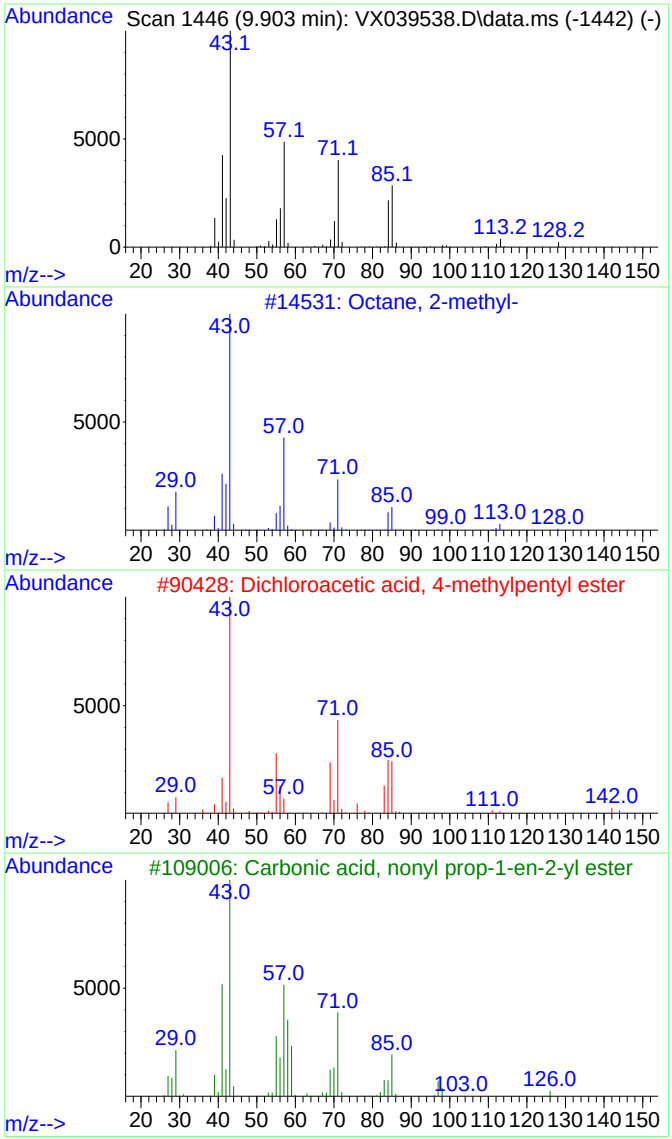
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

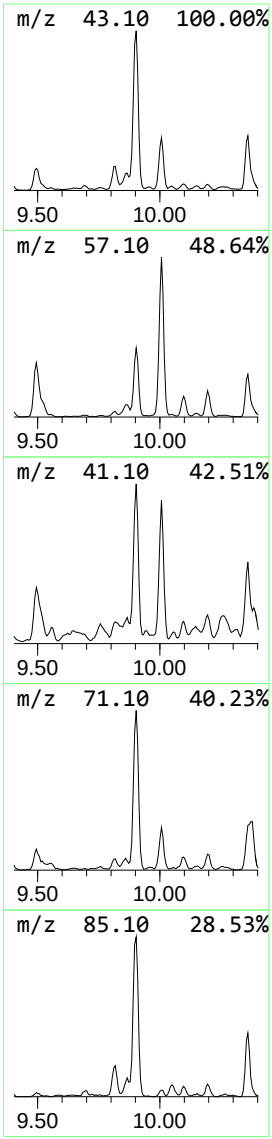
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Octane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.903	50.84 ug/l	573661	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	86
2	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	64
3	Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	64
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	59
5	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	53





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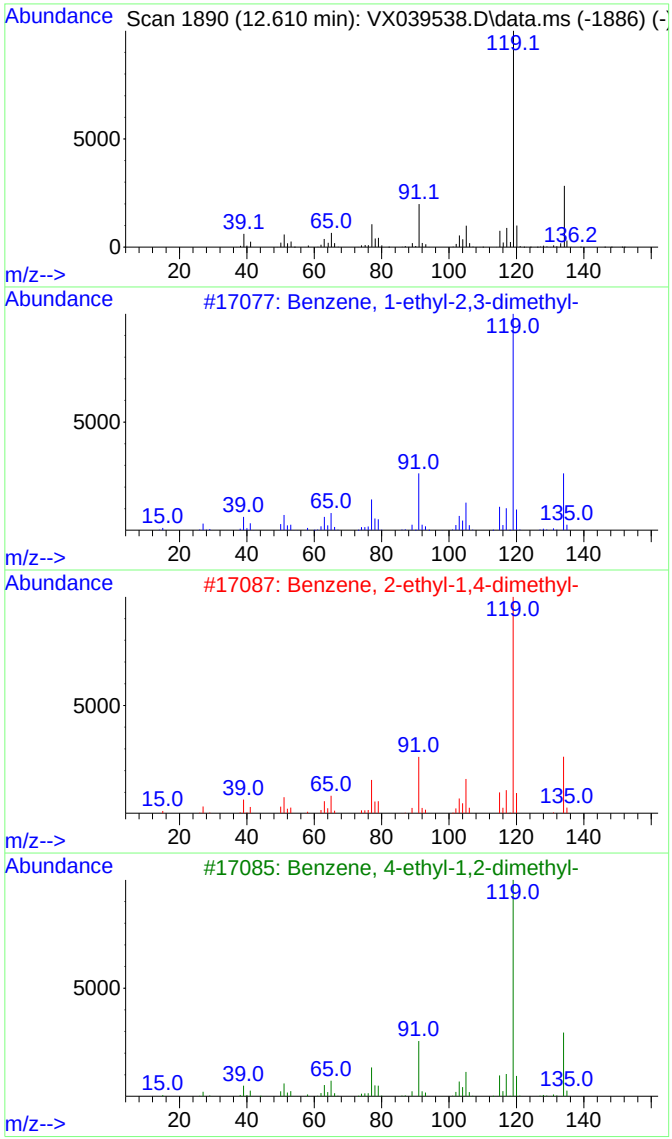
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

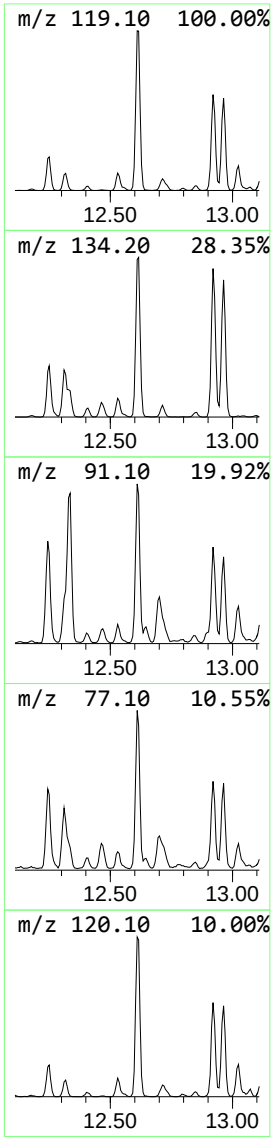
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	87.29 ug/l	1321040	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	p-Cymene	134	C10H14	000099-87-6	95





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Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

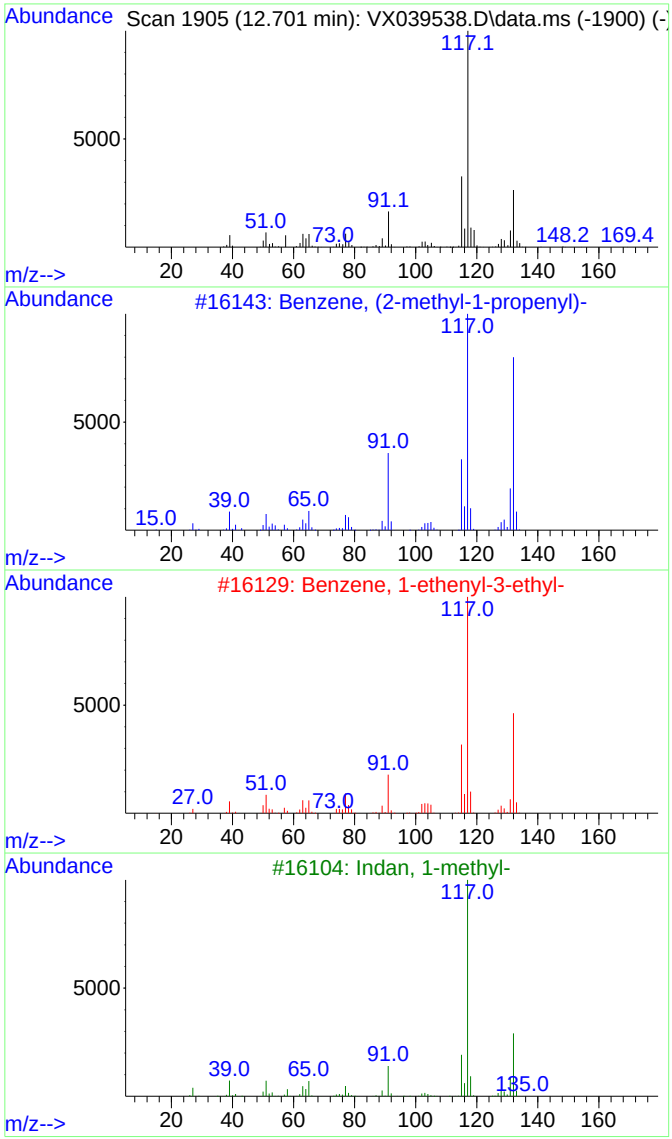
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

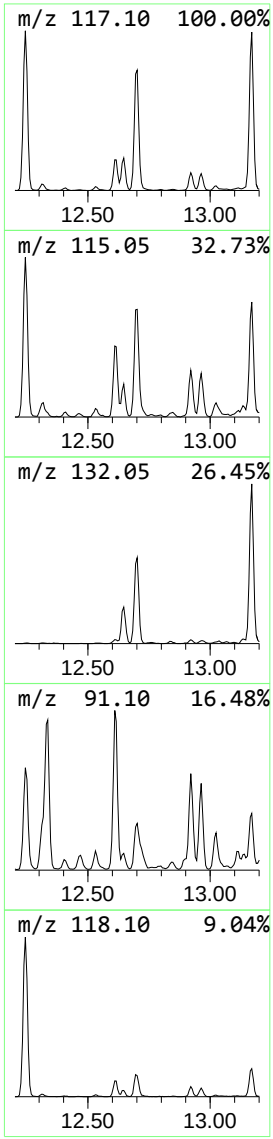
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	47.57 ug/l	719914	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122923\
Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
Sample : 06017-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

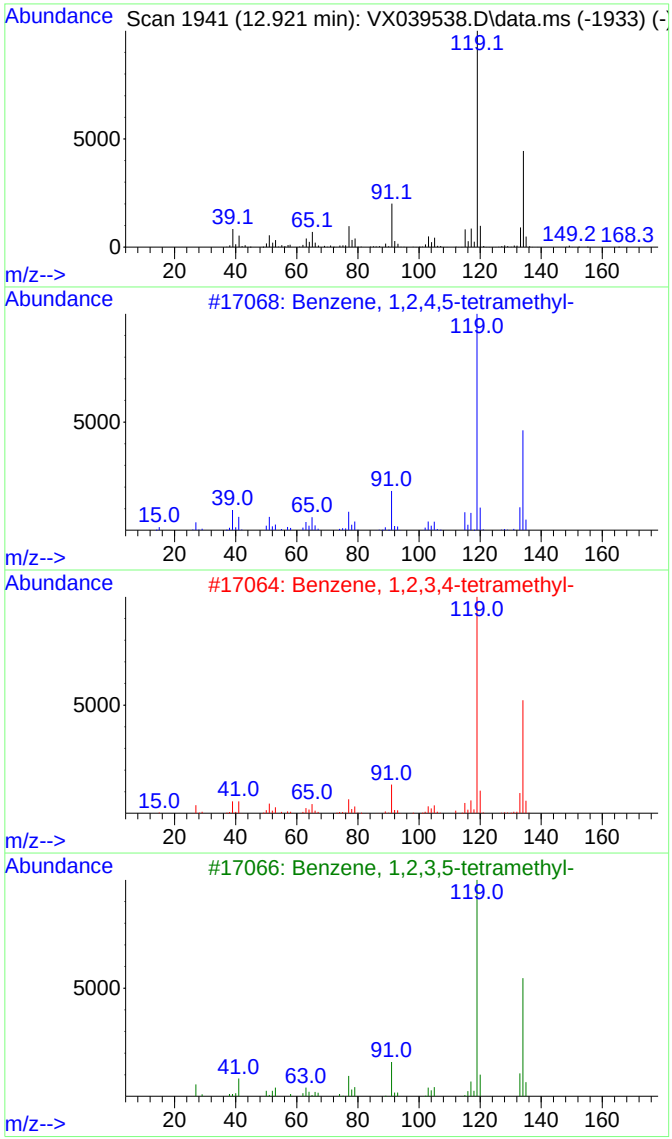
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

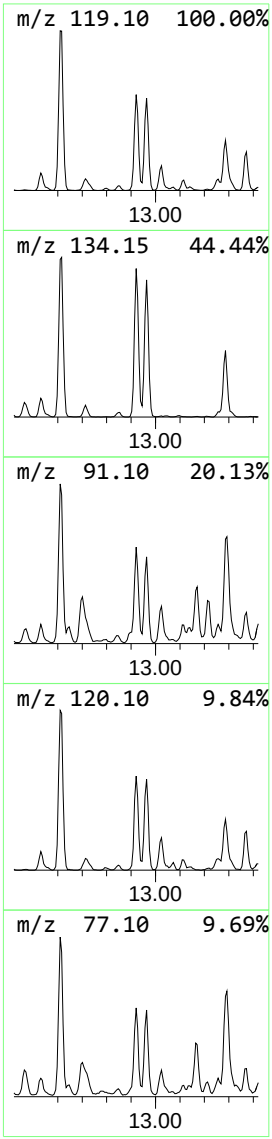
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	65.02 ug/l	983961	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122923\
Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
Sample : 06017-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

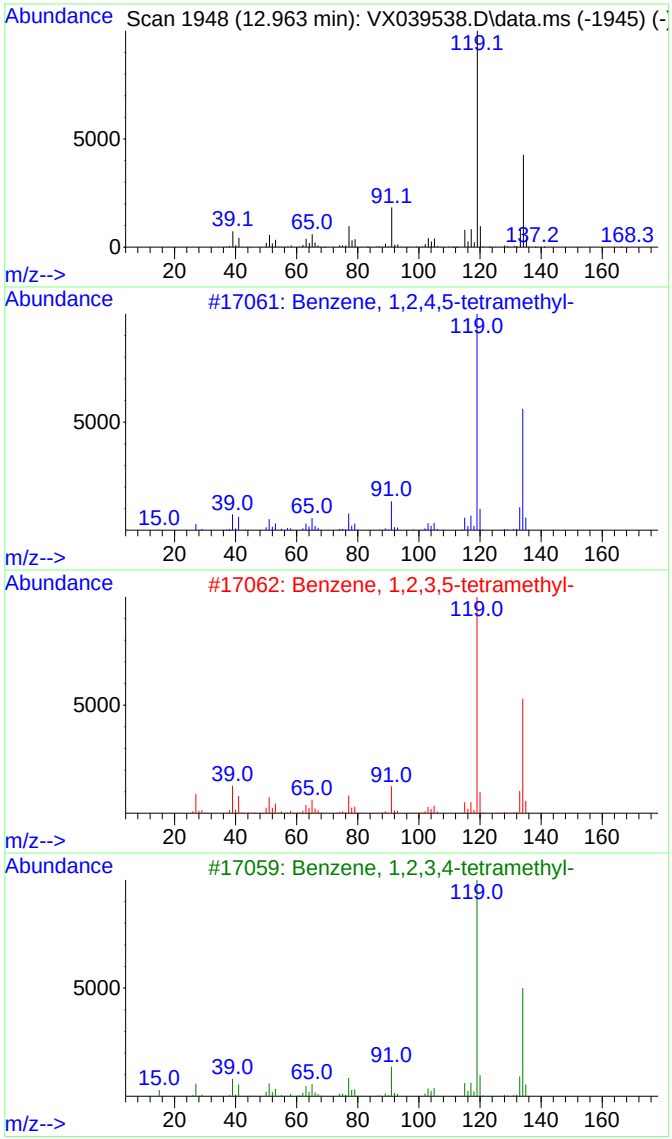
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

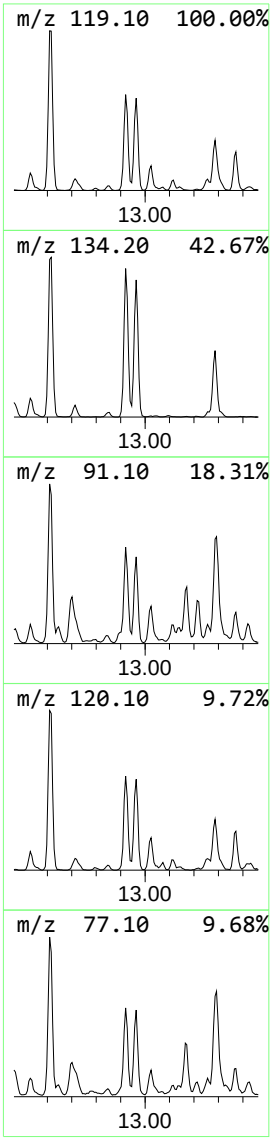
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	53.05 ug/l	802918	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122923\
Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
Sample : 06017-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

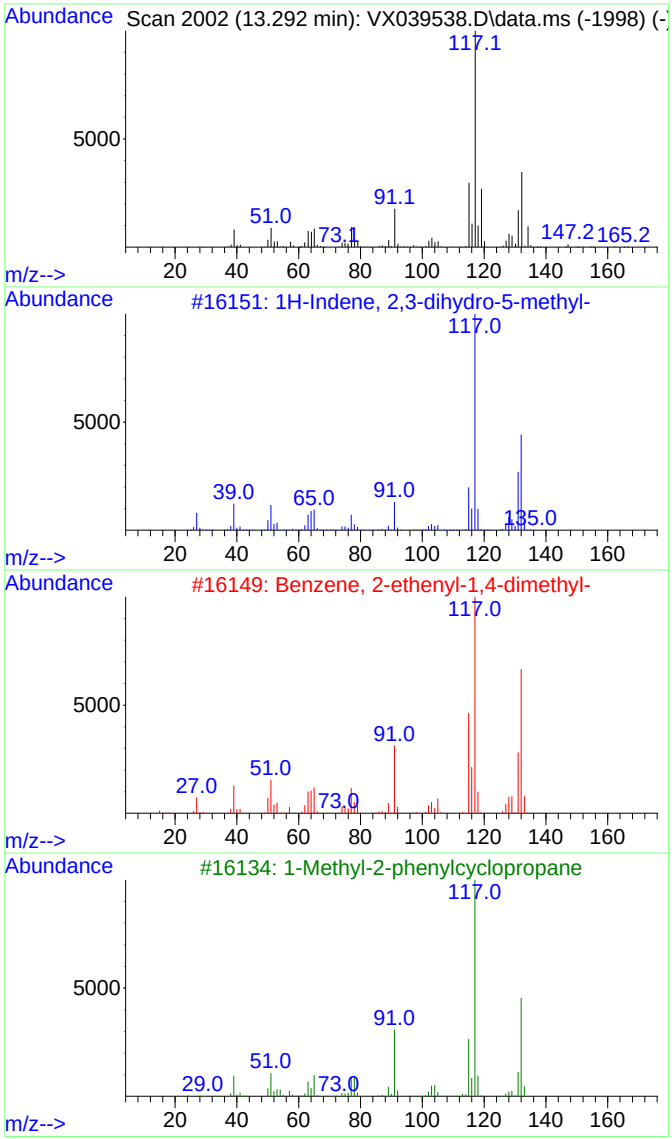
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

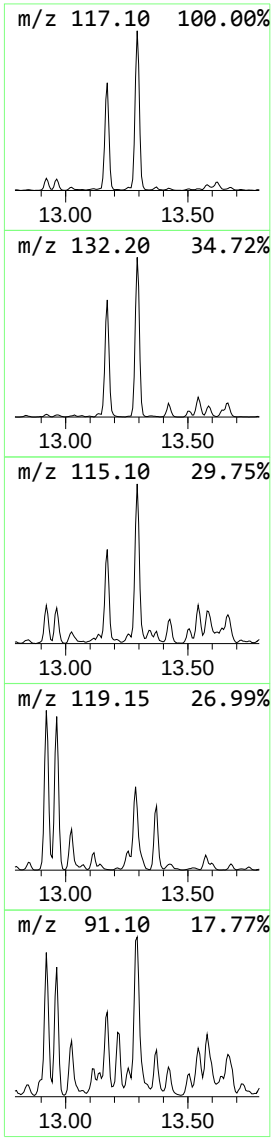
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	96.78 ug/l	1464740	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	81
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81





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Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
Sample : 06017-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

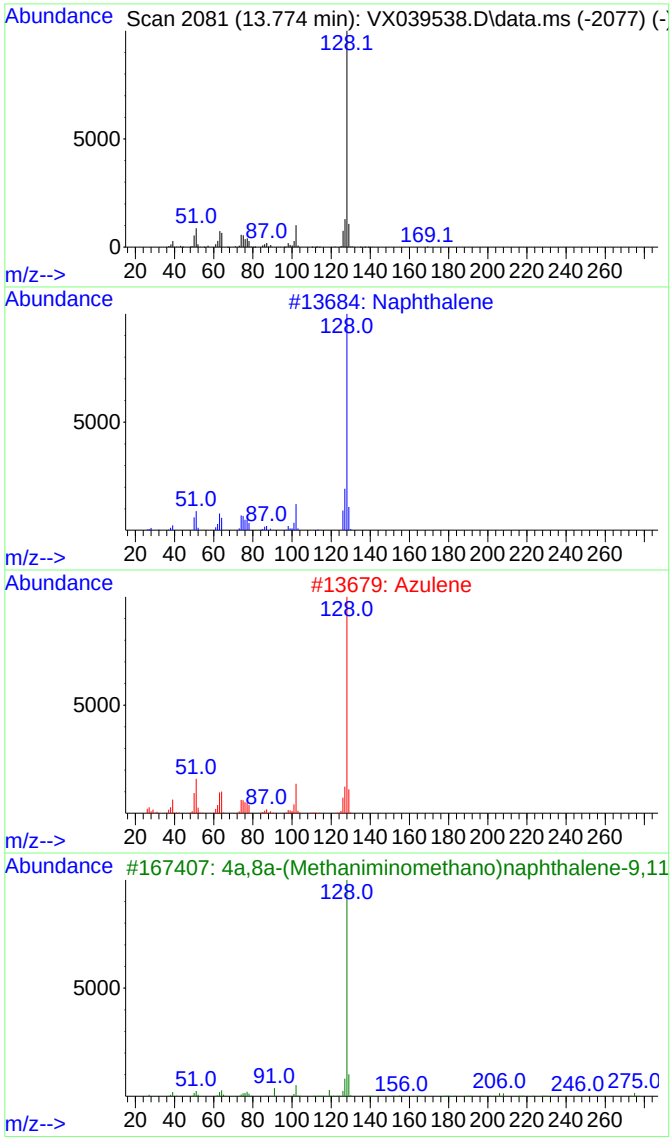
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

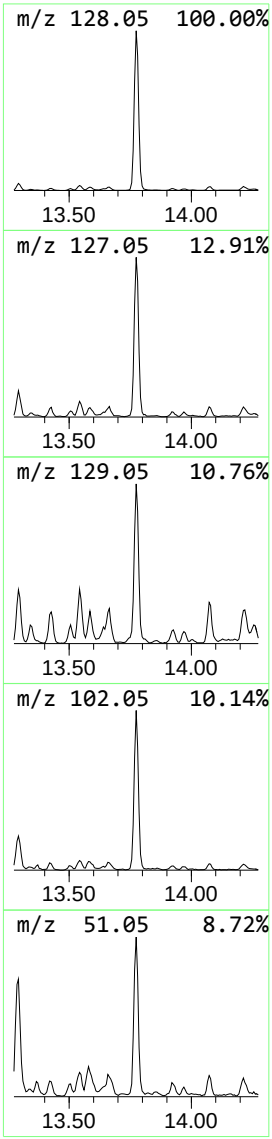
****

Peak Number 9 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	64.11 ug/l	970224	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	97
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	72
5	4-Fluorothiophenol	128	C6H5FS	000371-42-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122923\
Data File : VX039538.D
Acq On : 29 Dec 2023 12:27
Operator : JC/MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

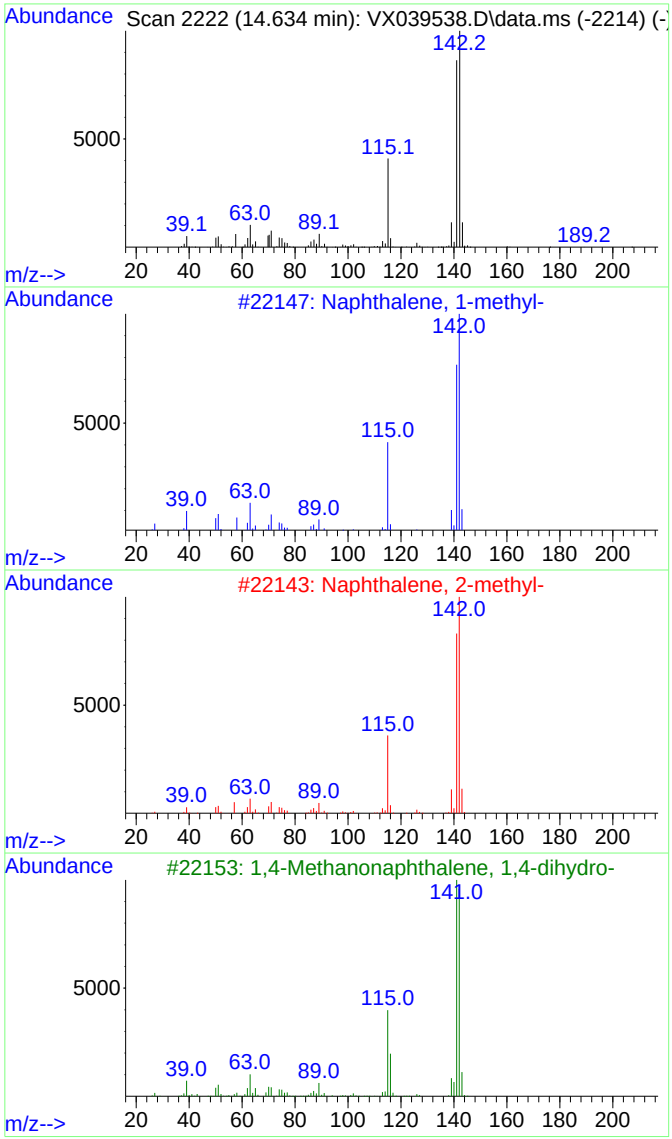
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

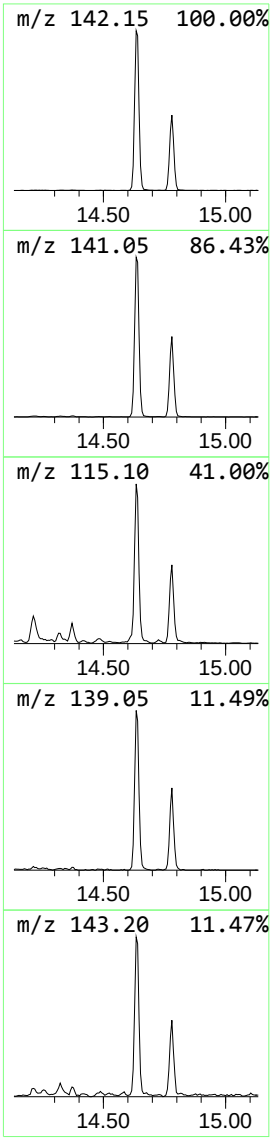
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	51.76 ug/l	783288	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
SB32-2-20231222-7.5-8.5-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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
Butane, 2,2,3,3...	6.233	42.5	ug/l	396414	2	6.763	466198	50.0
Octane, 2-methyl-	9.903	50.8	ug/l	573661	3	10.055	564140	50.0
Benzene, 1-ethy...	12.610	87.3	ug/l	1321040	4	12.024	756714	50.0
Benzene, (2-met...	12.701	47.6	ug/l	719914	4	12.024	756714	50.0
Benzene, 1,2,4,...	12.921	65.0	ug/l	983961	4	12.024	756714	50.0
Benzene, 1,2,3,...	12.963	53.0	ug/l	802918	4	12.024	756714	50.0
1H-Indene, 2,3-...	13.292	96.8	ug/l	1464740	4	12.024	756714	50.0
Azulene	13.774	64.1	ug/l	970224	4	12.024	756714	50.0
1,4-Methanonaph...	14.634	51.8	ug/l	783288	4	12.024	756714	50.0