LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.398	209	215	237	rBV	250355	588418	1.21%	0.072%
2	5.495	713	723	737	rVV2	731610	3042373	6.25%	0.372%
3	5.611	737	742	757	rVB2	214266	629709	1.29%	0.077%
4	5.812	762	775	789	rVV	898793	2618365	5.38%	0.320%
5	5.952	789	798	820	rVB	196048	530942	1.09%	0.065%
6	6.605	893	905	921	rBV	343618	836069	1.72%	0.102%
7	6.757	921	930	949	rVB	465932	1120676	2.30%	0.137%
8	8.647	1234	1240	1246	rBV	961028	1494713	3.07%	0.183%
9	8.714	1246	1251	1265	rVB	2222978	3431141	7.04%	0.419%
10	9.824	1427	1433	1437	rBV3	259794	543892	1.12%	0.066%
11	9.903	1442	1446	1451	rVB	605189	836223	1.72%	0.102%
12	10.006	1456	1463	1467	rBV	785242	1075394	2.21%	0.131%
13	10.055	1467	1471	1477	rVB	870853	1219336	2.50%	0.149%
14	10.195	1487	1494	1499	rBV	541327	950819	1.95%	0.116%
15	10.299	1499	1511	1517	rVV2	2437717	5305019	10.89%	0.648%
16	10.360	1517	1521	1532	rVB	4250412	5550786	11.39%	0.678%
17	10.458	1532	1537	1542	rBV	378544	579784	1.19%	0.071%
18	10.586	1551	1558	1562	rBV2	1115328	1766130	3.63%	0.216%
19	10.647	1564	1568	1570	rVV	932678	1250042	2.57%	0.153%
20	10.671	1570	1572	1575	rVB	457988	495676	1.02%	0.061%
21	10.781	1582	1590	1594	rBV	4210543	6274880	12.88%	0.766%
22	10.854	1594	1602	1606	rVV3	3506413	6744583	13.85%	0.824%
23	10.896	1606	1609	1614	rVV	2517984	3623013	7.44%	0.442%
24	10.951	1614	1618	1623	rVV3	1241551	2341194	4.81%	0.286%
25	11.000	1623	1626	1628	rVV2	1237399	1621838	3.33%	0.198%
26	11.031	1628	1631	1634	rVV	2067997	2846006	5.84%	0.348%
27	11.085	1634	1640	1643	rVV2	5354237	9242480	18.97%	1.129%
28	11.110	1643	1644	1650	rVB2	3791756	3795996	7.79%	0.464%
29	11.195	1650	1658	1660	rBV	4705717	7811908	16.04%	0.954%
30	11.220	1660	1662	1670	rVV3	5297999	7068280	14.51%	0.863%
31	11.311	1673	1677	1679	rVV	1997775	3141928	6.45%	0.384%
32	11.342	1679	1682	1685	rVV2	2504116	4278968	8.78%	0.523%
33	11.384	1685	1689	1694	rVV	7668059	15120705	31.04%	1.846%
34	11.433	1694	1697	1699	rVV	8927819	12420100	25.50%	1.517%
35	11.482	1701	1705	1710	rVV	27740938	40467869	83.07%	4.942%
36	11.524	1710	1712	1715	rVV3	1556688	2032696	4.17%	0.248%

LSC Area Percent Report

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Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

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\82X031023W.M
Title : SW846 8260

37	11.579	1717	1721	1723	rVV2	1581944	2704559	5.55%	0.330%
38	11.622	1723	1728	1734	rVV3	5822094	13417869	27.54%	1.639%
39	11.689	1734	1739	1741	rVV4	2530292	4100280	8.42%	0.501%
40	11.720	1741	1744	1747	rVV	10979935	14451802	29.67%	1.765%
41	11.762	1747	1751	1759	rVV	21942402	35824394	73.54%	4.375%
42	11.848	1759	1765	1766	rVV2	2132060	3437736	7.06%	0.420%
43	11.896	1766	1773	1777	rVV4	9388432	19824269	40.70%	2.421%
44	11.951	1777	1782	1784	rVV	12906217	19390978	39.81%	2.368%
45	11.976	1784	1786	1790	rVV2	9031269	12395046	25.45%	1.514%
46	12.018	1790	1793	1795	rVV	4865492	7708556	15.82%	0.941%
47	12.043	1795	1797	1800	rVV	6167906	8160940	16.75%	0.997%
48	12.097	1800	1806	1812	rVV3	16323906	33898191	69.59%	4.139%
49	12.177	1812	1819	1826	rVB4	6285481	13922781	28.58%	1.700%
50	12.274	1832	1835	1838	rVB	12360073	14853045	30.49%	1.814%
51	12.323	1838	1843	1849	rVB3	21927516	42011952	86.24%	5.130%
52	12.433	1849	1861	1864	rBV2	32412444	48712700	100.00%	5.949%
53	12.469	1864	1867	1873	rVB2	13817802	19778009	40.60%	2.415%
54	12.543	1874	1879	1880	rBV	9264460	12622794	25.91%	1.541%
55	12.561	1880	1882	1886	rVV	11181434	14003855	28.75%	1.710%
56	12.622	1889	1892	1895	rVB	9100455	9974043	20.48%	1.218%
57	12.732	1900	1910	1914	rBV6	11712138	32656422	67.04%	3.988%
58	12.768	1914	1916	1918	rBV3	1780466	1850289	3.80%	0.226%
59	12.805	1918	1922	1923	rBV2	4146279	4942285	10.15%	0.604%
60	12.829	1923	1926	1928	rBV	2557866	2227930	4.57%	0.272%
61	12.853	1928	1930	1933	rVB2	5957013	5682137	11.66%	0.694%
62	12.896	1933	1937	1940	rBV3	10103437	17757412	36.45%	2.168%
63	12.969	1945	1949	1955	rVV	17854820	33363420	68.49%	4.074%
64	13.030	1955	1959	1960	rVV	7595789	9428126	19.35%	1.151%
65	13.073	1964	1966	1969	rVV	5705054	8020434	16.46%	0.979%
66	13.103	1969	1971	1975	rVV2	4460799	7245742	14.87%	0.885%
67	13.164	1975	1981	1985	rVV4	10072554	20096728	41.26%	2.454%
68	13.219	1986	1990	1993	rVV	9157809	12333159	25.32%	1.506%
69	13.262	1993	1997	1999	rVV3	9720788	17325758	35.57%	2.116%
70	13.292	1999	2002	2007	rVV2	27874466	44574177	91.50%	5.443%
71	13.335	2007	2009	2013	rVV	6628387	8380640	17.20%	1.023%
72	13.372	2013	2015	2018	rVV	5005330	6235896	12.80%	0.761%
73	13.427	2021	2024	2033	rVB2	10118942	18290616	37.55%	2.234%
74	13.512	2033	2038	2040	rBV2	3627735	5427569	11.14%	0.663%
75	13.542	2040	2043	2046	rVV3	2747495	3791998	7.78%	0.463%
76	13.585	2046	2050	2055	rVV2	7734898	15508224	31.84%	1.894%

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Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

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\82X031023W.M
Title : SW846 8260

77	13.628	2055	2057	2061	rVV5	2814071	5588175	11.47%	0.682%
78	13.670	2061	2064	2069	rVB2	4334694	6869462	14.10%	0.839%
79	13.756	2074	2078	2079	rVV	1533672	1884973	3.87%	0.230%
80	13.780	2079	2082	2088	rVV2	5002329	8639788	17.74%	1.055%
81	13.853	2088	2094	2099	rVB4	1290459	2539378	5.21%	0.310%
82	13.902	2099	2102	2104	rBV2	943104	1227506	2.52%	0.150%
83	13.926	2104	2106	2111	rVB3	1382428	1863397	3.83%	0.228%
84	13.975	2111	2114	2117	rVB	450740	530924	1.09%	0.065%
85	14.231	2149	2156	2161	rVB3	338643	728318	1.50%	0.089%

Sum of corrected areas: 818902633

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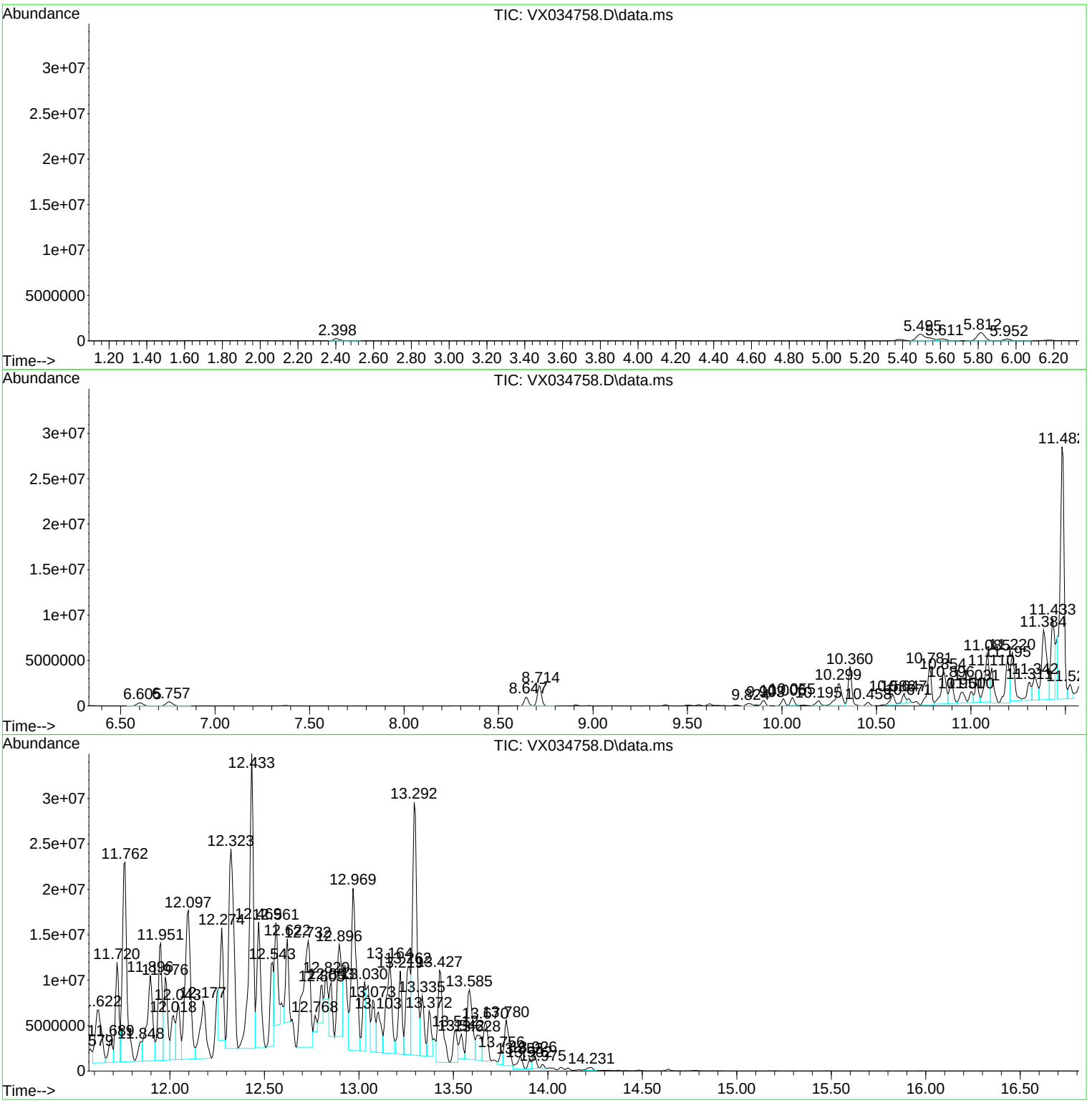
Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
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Operator : JC/MD
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

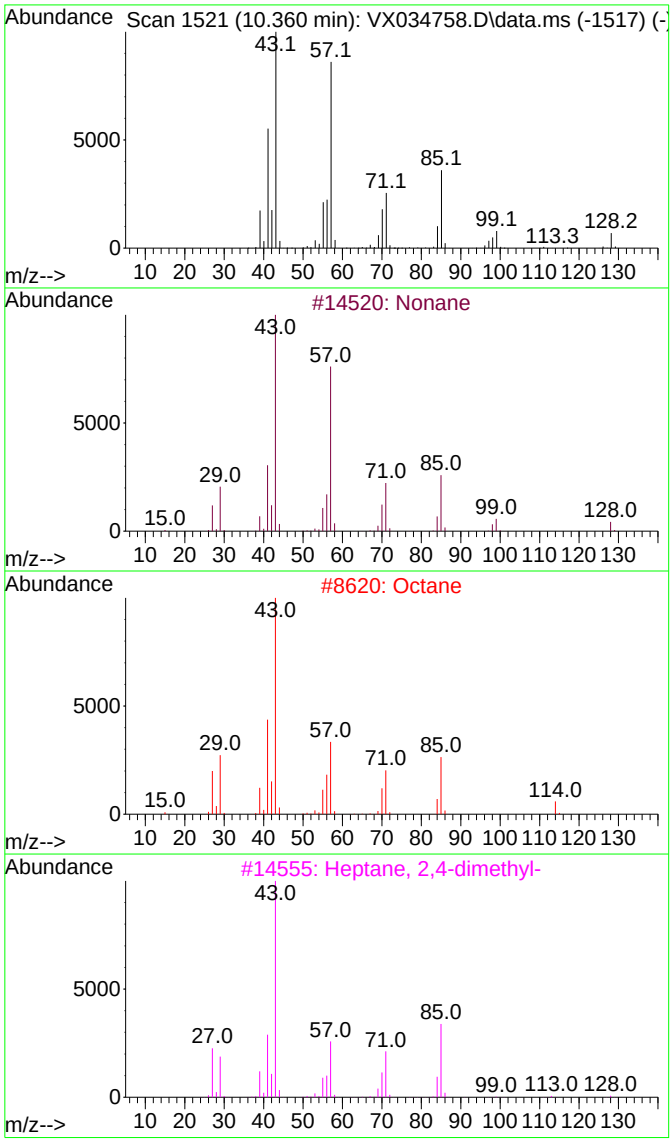
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

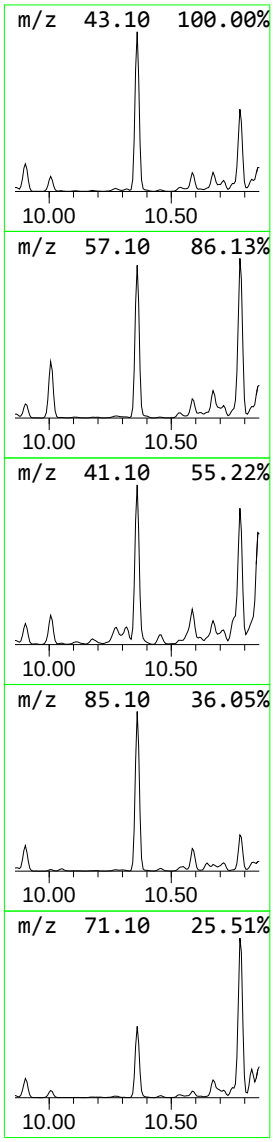
****

Peak Number 1 Nonane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	227.62 ug/l	5550790	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	97
2	Octane	114	C8H18	000111-65-9	64
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
4	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	53
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

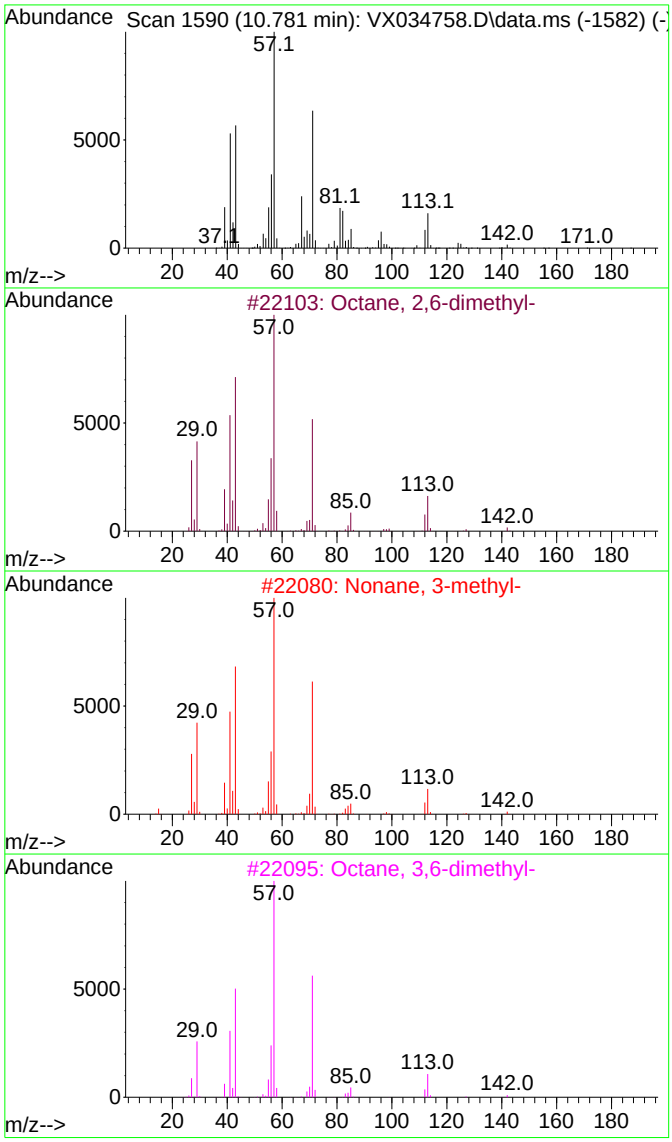
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

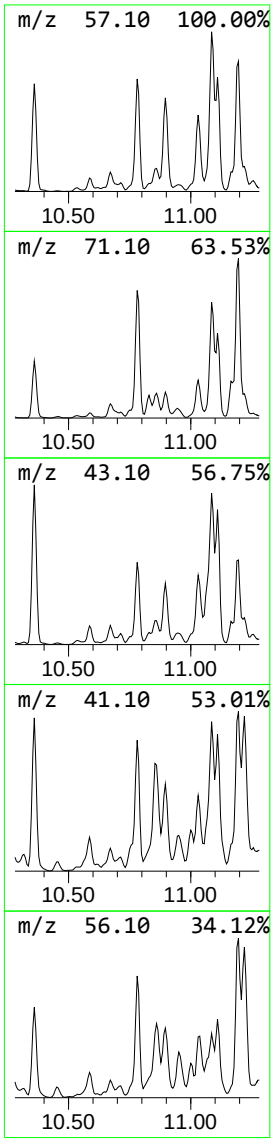
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	257.31 ug/l	6274880	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	76
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	76
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	68
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	50
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	49





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MSVOA_X
ClientSampleId :
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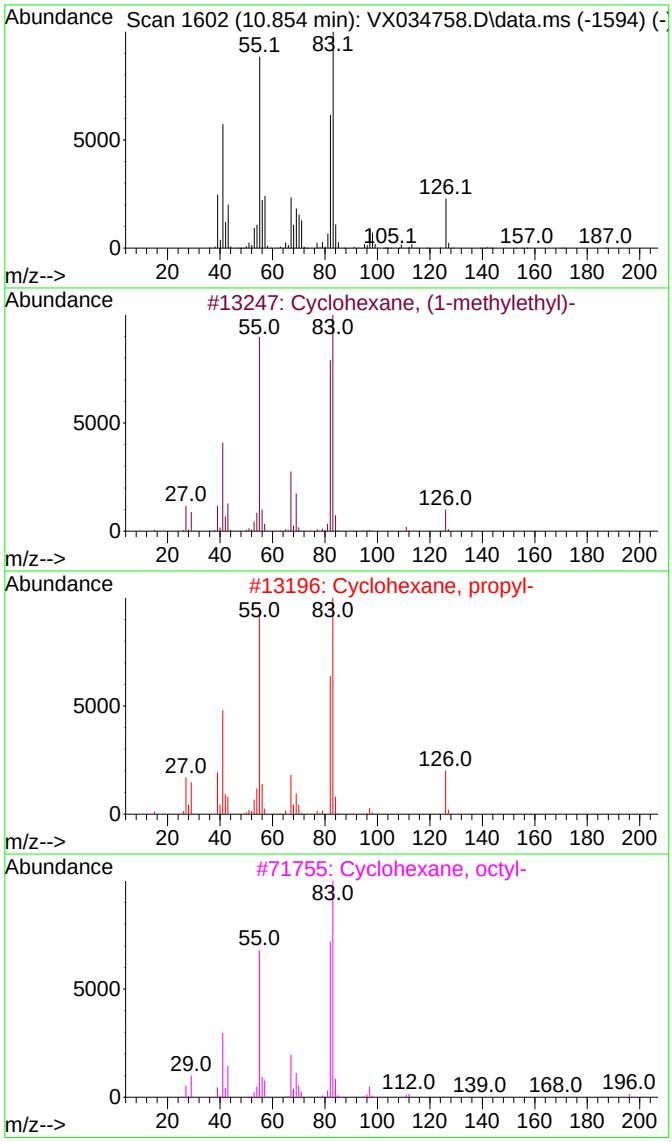
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

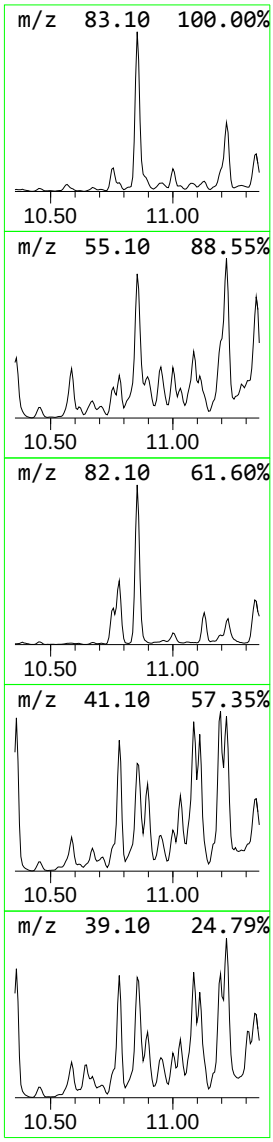
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, (1-methylethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	276.57 ug/l	6744580	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	87
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	64
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	64
5	2,3-Dimethyl-2-heptene	126	C9H18	003074-64-4	53





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Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

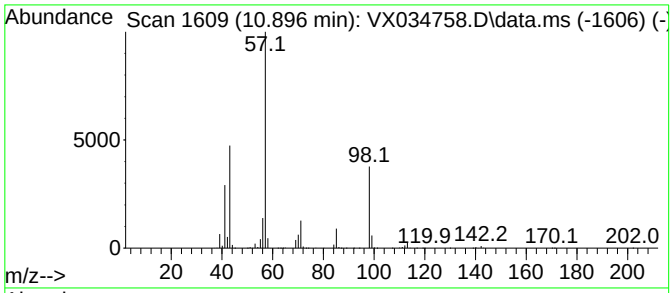
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

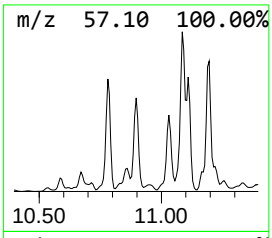
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

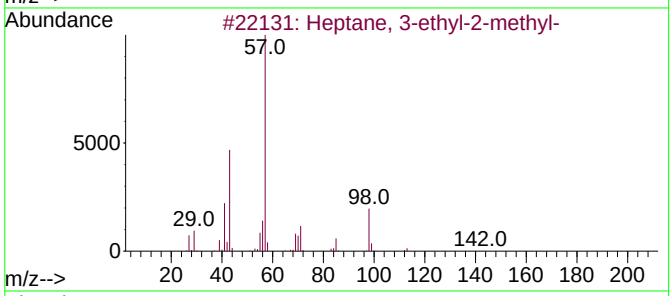
****
Peak Number 4 Heptane, 3-ethyl-2-methyl- Concentration Rank 9

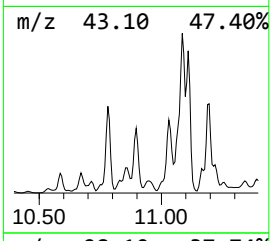
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.897	148.57 ug/l	3623010	Chlorobenzene-d5	10.055

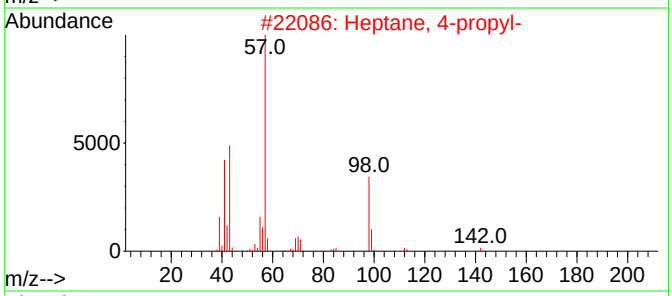
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	83
2	Heptane, 4-propyl-	142	C10H22	003178-29-8	64
3	Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	59
4	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	53
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50

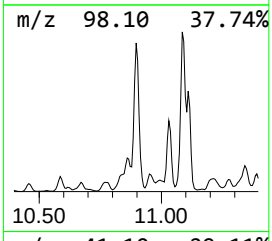


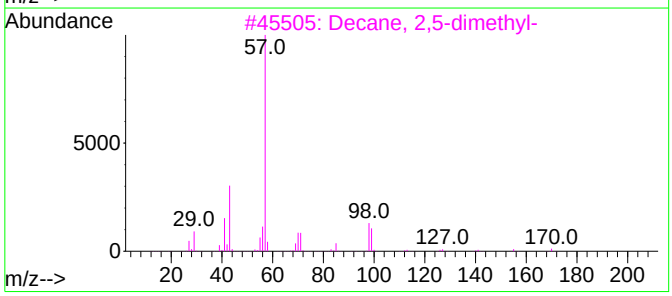


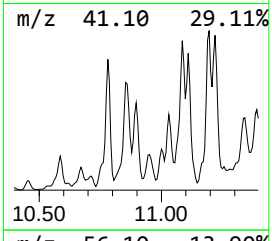


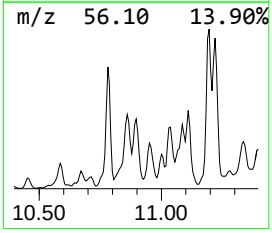












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Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

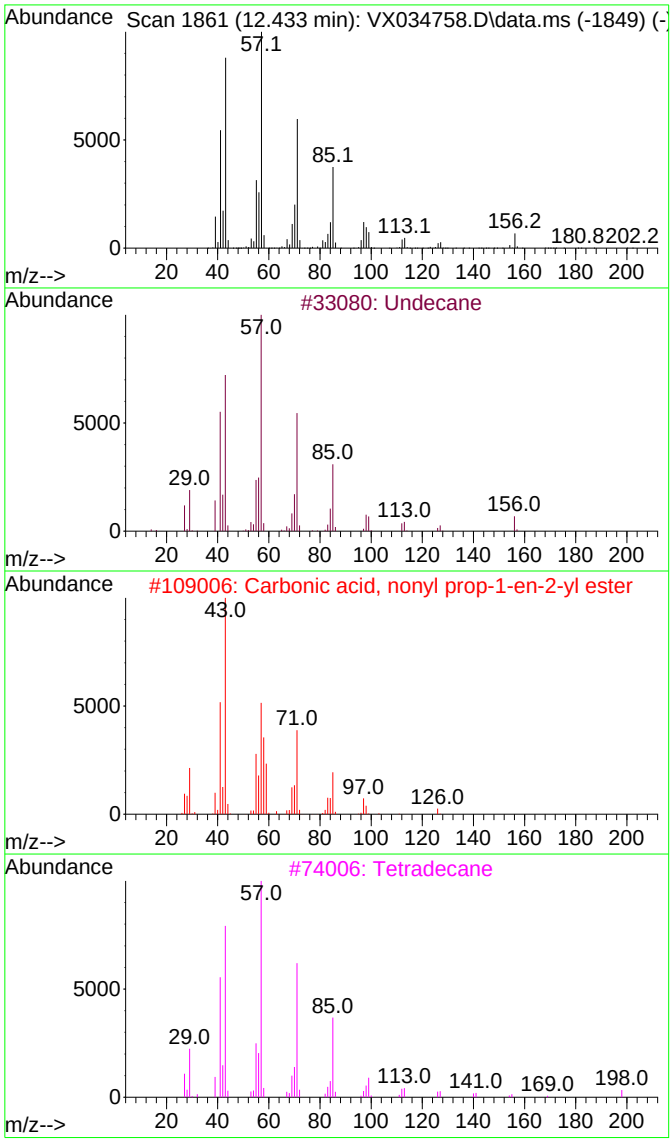
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

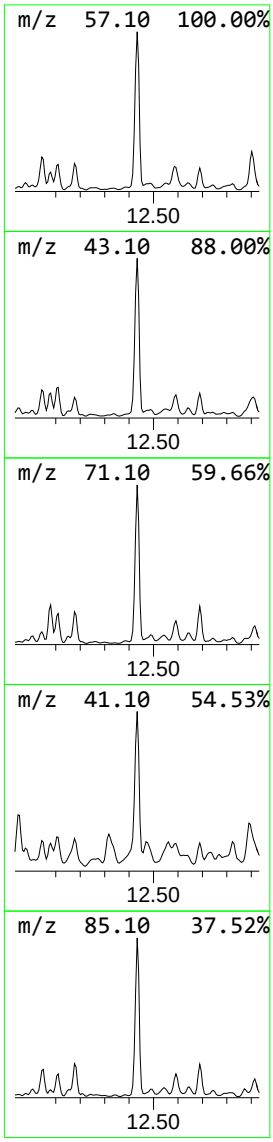
****

Peak Number 6 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	298.45 ug/l	48712700	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	86
3	Tetradecane	198	C14H30	000629-59-4	64
4	1-Decene, 4-methyl-	154	C11H22	013151-29-6	49
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

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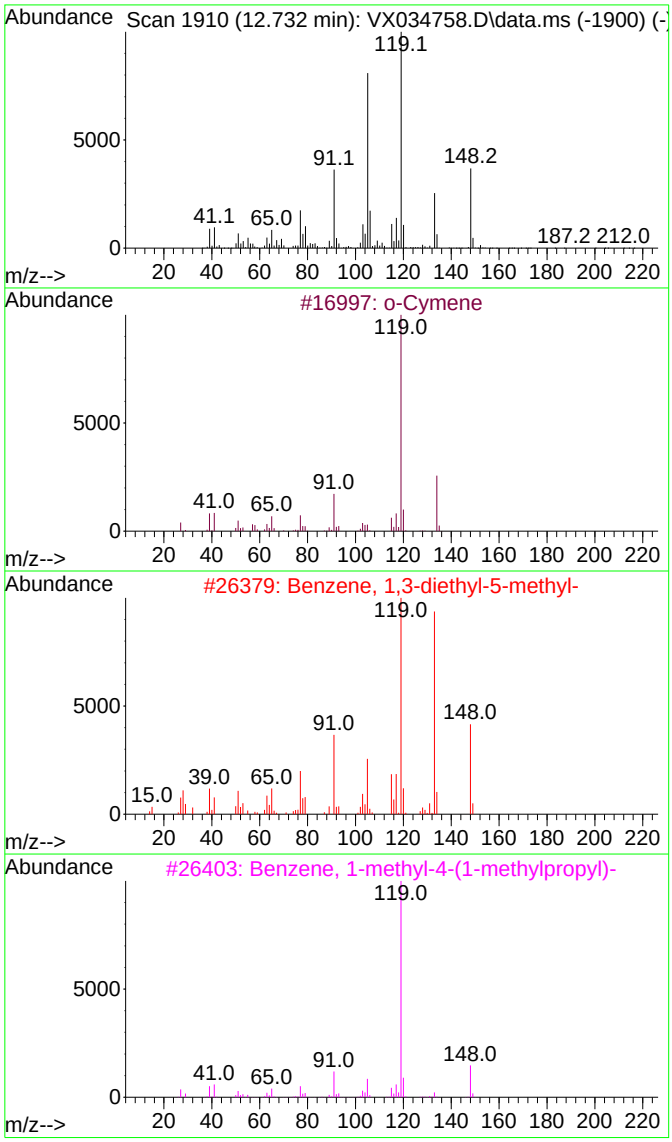
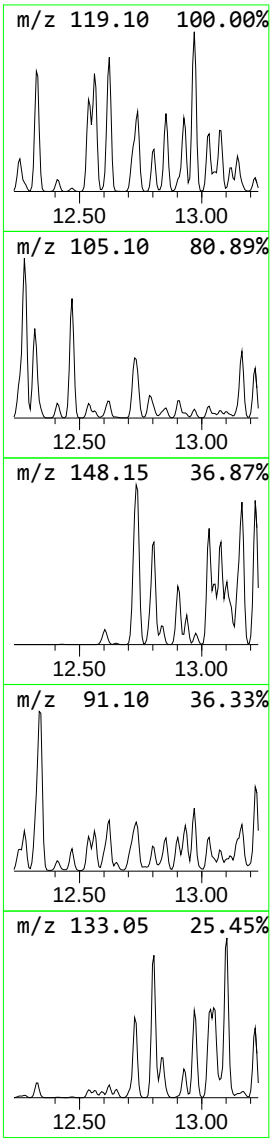
Peak Number 7 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.732	200.08 ug/l	32656400	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	90
2	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	72
3	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	64
4	1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	62
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

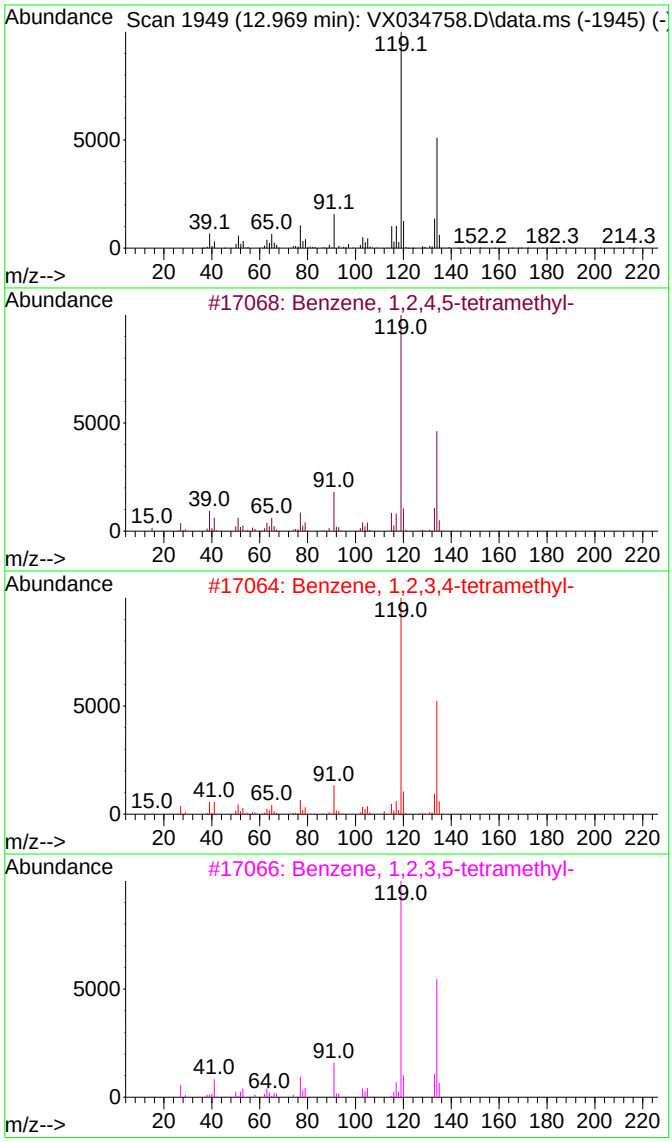
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

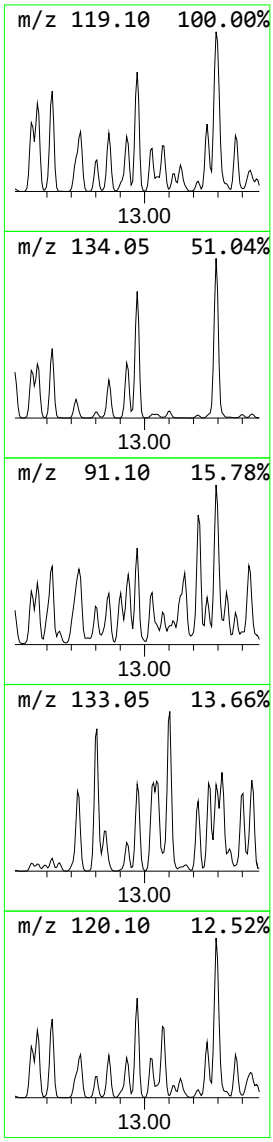
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	204.41 ug/l	33363400	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

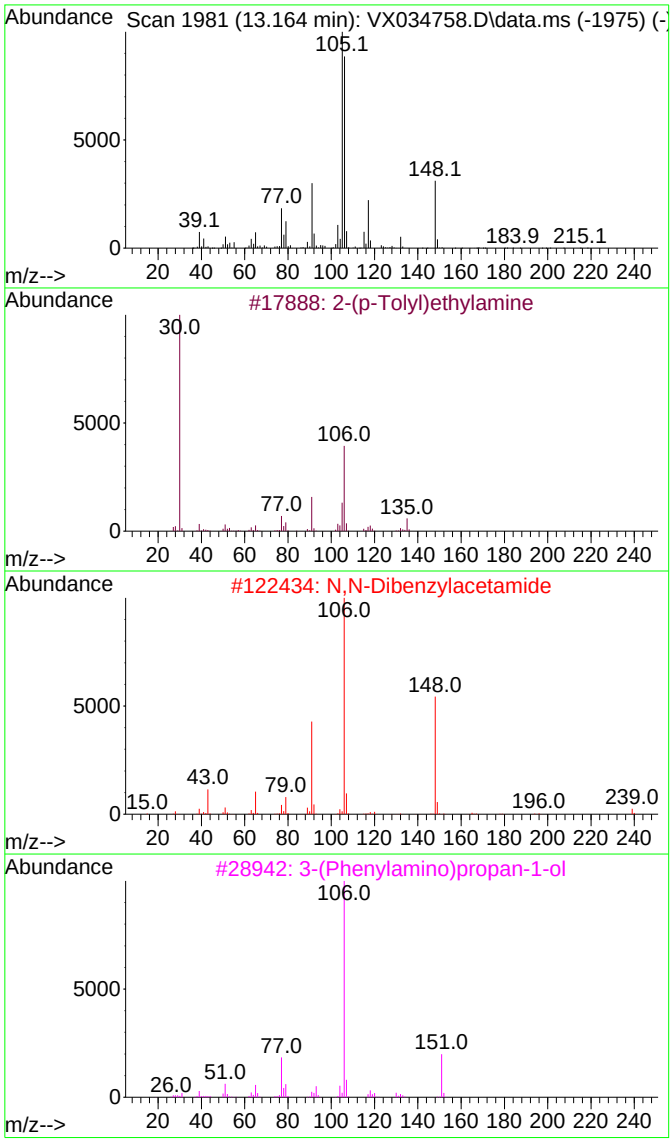
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

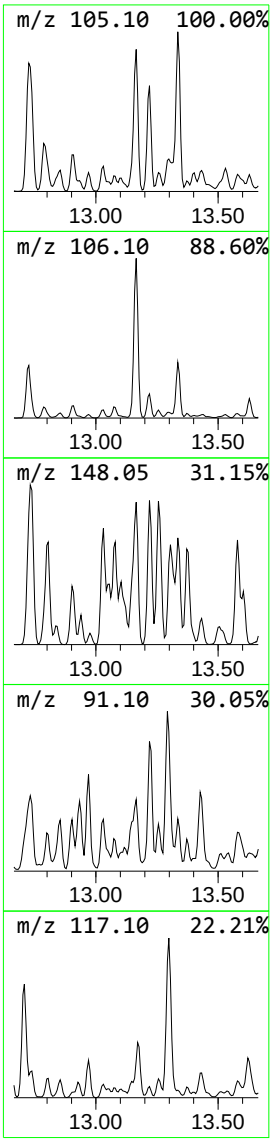
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-(p-Tolyl)ethylamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	123.13 ug/l	20096700	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	59
2	N,N-Dibenzylacetamide	239	C16H17NO	010479-30-8	50
3	3-(Phenylamino)propan-1-ol	151	C9H13NO	1000484-17-7	43
4	2-Amino-2-phenylethyl benzoate	241	C15H15NO2	496871-35-3	43
5	Benzenamine, N-propyl-	135	C9H13N	000622-80-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
Sample : 02052-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

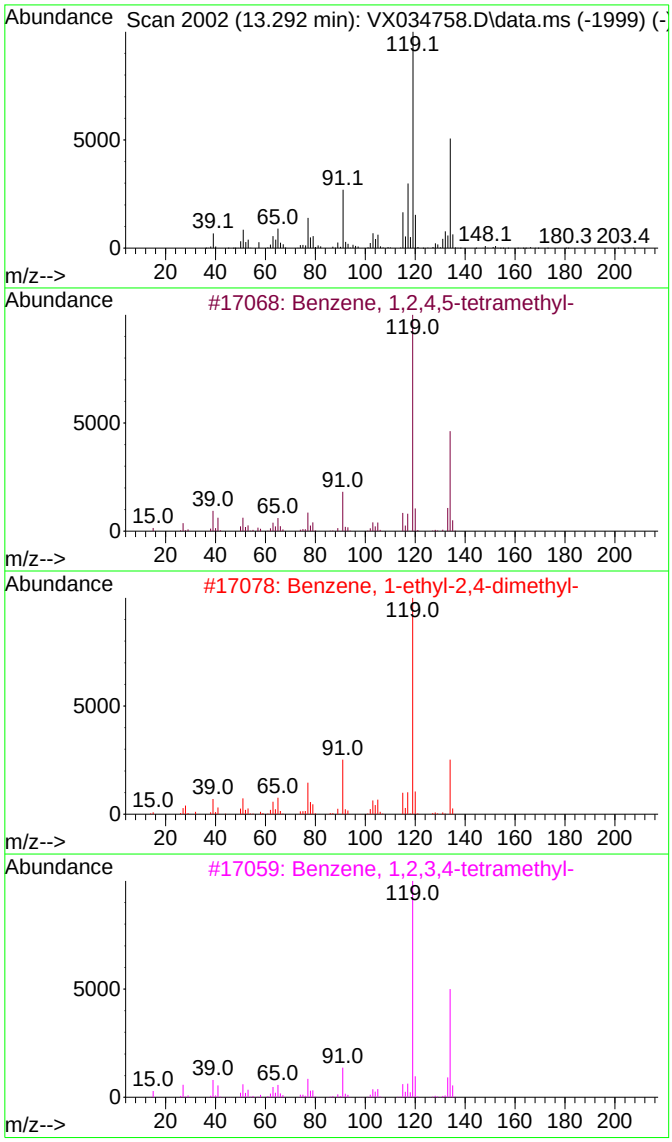
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

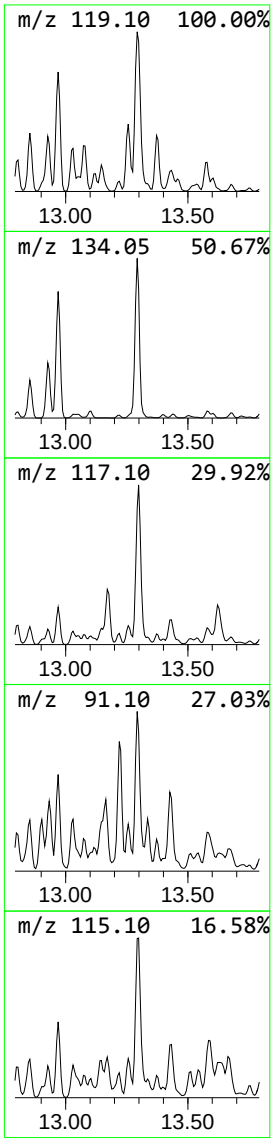
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	273.10 ug/l	44574200	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	90
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	90
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	80
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032723\
Data File : VX034758.D
Acq On : 27 Mar 2023 18:31
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
AUD-1846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
Nonane	10.360	227.6	ug/l	5550790	3	10.055	1219340	50.0
Octane, 2,6-dim...	10.781	257.3	ug/l	6274880	3	10.055	1219340	50.0
Cyclohexane, (1...	10.854	276.6	ug/l	6744580	3	10.055	1219340	50.0
Heptane, 3-ethy...	10.897	148.6	ug/l	3623010	3	10.055	1219340	50.0
Undecane	12.433	298.4	ug/l	48712700	4	12.030	8160940	50.0
o-Cymene	12.732	200.1	ug/l	32656400	4	12.030	8160940	50.0
Benzene, 1,2,4,...	12.969	204.4	ug/l	33363400	4	12.030	8160940	50.0
2-(p-Tolyl)ethy...	13.164	123.1	ug/l	20096700	4	12.030	8160940	50.0
Benzene, 1-ethy...	13.292	273.1	ug/l	44574200	4	12.030	8160940	50.0