LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

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\82X051921W.M
Title : SW846 8260

Signal : TIC: VX022234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.892	128	132	142	rVB	29594	39926	1.32%	0.156%
2	2.745	263	272	275	rBV	32924	71220	2.35%	0.279%
3	2.788	275	279	298	rVB	90271	202855	6.70%	0.794%
4	3.068	317	325	334	rBV	64372	144099	4.76%	0.564%
5	3.416	373	382	396	rBV	70703	157291	5.20%	0.616%
6	4.190	499	509	516	rBV2	41301	117242	3.87%	0.459%
7	4.281	516	524	537	rVB2	83078	233513	7.71%	0.914%
8	5.111	648	660	668	rBV3	9988	40848	1.35%	0.160%
9	5.397	691	707	711	rBV	48959	142626	4.71%	0.558%
10	5.482	711	721	728	rVV5	106731	457950	15.13%	1.792%
11	5.556	728	733	737	rVV	83301	224249	7.41%	0.878%
12	5.604	738	741	760	rVV	83827	229942	7.60%	0.900%
13	5.812	763	775	789	rVV2	121177	367891	12.15%	1.440%
14	5.964	789	800	807	rVV	60718	163552	5.40%	0.640%
15	6.037	807	812	820	rVV2	20055	51961	1.72%	0.203%
16	6.147	820	830	836	rVV3	51197	165278	5.46%	0.647%
17	6.238	836	845	856	rVV	408524	1259332	41.61%	4.928%
18	6.348	856	863	877	rVB2	55114	161134	5.32%	0.631%
19	6.604	895	905	915	rBV2	74688	179541	5.93%	0.703%
20	6.763	922	931	939	rBV	135741	357354	11.81%	1.398%
21	6.848	940	945	955	rVB5	35020	92851	3.07%	0.363%
22	7.061	973	980	989	rBV5	12240	30994	1.02%	0.121%
23	7.165	990	997	1004	rBV2	20131	43202	1.43%	0.169%
24	7.378	1016	1032	1043	rBV	331709	821955	27.16%	3.216%
25	7.494	1043	1051	1056	rBV	87773	178698	5.90%	0.699%
26	7.561	1056	1062	1066	rVV	93321	206764	6.83%	0.809%
27	7.598	1066	1068	1073	rVV2	46704	84063	2.78%	0.329%
28	7.653	1073	1077	1084	rVB2	55731	107273	3.54%	0.420%
29	7.775	1090	1097	1104	rVB2	42571	87929	2.91%	0.344%
30	7.982	1121	1131	1143	rVB	441910	922747	30.49%	3.611%
31	8.104	1143	1151	1160	rBV2	583204	1276294	42.17%	4.994%
32	8.189	1160	1165	1174	rVV2	120518	254392	8.40%	0.995%
33	8.275	1174	1179	1182	rVV	91891	156339	5.17%	0.612%
34	8.311	1182	1185	1191	rVV5	67026	119725	3.96%	0.469%
35	8.384	1191	1197	1201	rVV	28300	54461	1.80%	0.213%
36	8.439	1201	1206	1210	rVV	98261	178258	5.89%	0.698%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

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\82X051921W.M
Title : SW846 8260

37	8.506	1213	1217	1226	rVB4	43133	89237	2.95%	0.349%
38	8.610	1226	1234	1237	rBV3	221716	482598	15.94%	1.888%
39	8.653	1237	1241	1249	rVB	314656	537988	17.77%	2.105%
40	8.775	1256	1261	1265	rBV	54387	79277	2.62%	0.310%
41	8.817	1265	1268	1270	rVV2	29580	38501	1.27%	0.151%
42	8.848	1270	1273	1278	rVB	38986	58335	1.93%	0.228%
43	8.921	1278	1285	1290	rBV4	49416	99936	3.30%	0.391%
44	8.976	1290	1294	1301	rVB2	84621	138917	4.59%	0.544%
45	9.104	1306	1315	1320	rBV	73438	141767	4.68%	0.555%
46	9.165	1320	1325	1328	rVV	61308	96181	3.18%	0.376%
47	9.201	1328	1331	1337	rVB2	41075	60128	1.99%	0.235%
48	9.384	1355	1361	1366	rBV2	50363	82221	2.72%	0.322%
49	9.506	1376	1381	1386	rBV4	77682	158416	5.23%	0.620%
50	9.567	1386	1391	1394	rVB	90594	124338	4.11%	0.487%
51	9.616	1394	1399	1404	rBV2	69507	120533	3.98%	0.472%
52	9.659	1404	1406	1417	rVB6	25973	55931	1.85%	0.219%
53	9.762	1417	1423	1428	rBV4	32483	57574	1.90%	0.225%
54	9.829	1428	1434	1438	rBV5	43369	97156	3.21%	0.380%
55	9.902	1443	1446	1451	rVB	83493	121879	4.03%	0.477%
56	10.012	1456	1464	1467	rBV	79698	112226	3.71%	0.439%
57	10.061	1467	1472	1476	rBV	267263	373364	12.34%	1.461%
58	10.104	1476	1479	1482	rBV	40330	56415	1.86%	0.221%
59	10.201	1490	1495	1499	rVB5	48031	80406	2.66%	0.315%
60	10.305	1499	1512	1518	rVV	2148129	3026812	100.00%	11.844%
61	10.378	1518	1524	1533	rVB4	35807	99490	3.29%	0.389%
62	10.463	1533	1538	1547	rBV4	17325	32121	1.06%	0.126%
63	10.585	1552	1558	1563	rBV3	56131	97666	3.23%	0.382%
64	10.646	1565	1568	1571	rBV	28777	32385	1.07%	0.127%
65	10.780	1587	1590	1594	rVB2	52970	69611	2.30%	0.272%
66	10.860	1599	1603	1607	rVV3	39537	55934	1.85%	0.219%
67	10.963	1615	1620	1625	rBV	124963	172935	5.71%	0.677%
68	11.085	1635	1640	1644	rBV	241840	329964	10.90%	1.291%
69	11.122	1644	1646	1651	rVB	112076	135582	4.48%	0.531%
70	11.195	1651	1658	1660	rBV2	24648	33530	1.11%	0.131%
71	11.311	1666	1677	1684	rVV	287694	407189	13.45%	1.593%
72	11.384	1684	1689	1695	rVV	1197468	1480376	48.91%	5.793%
73	11.457	1695	1701	1714	rVB	754800	949626	31.37%	3.716%
74	11.616	1722	1727	1735	rVB	532155	658044	21.74%	2.575%
75	11.756	1745	1750	1759	rVB	2163852	2570841	84.94%	10.060%
76	11.847	1760	1765	1767	rBV	22498	32500	1.07%	0.127%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

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\82X051921W.M
Title : SW846 8260

77	11.939	1776	1780	1783	rBV	75699	99609	3.29%	0.390%
78	11.975	1783	1786	1789	rVB	35962	40019	1.32%	0.157%
79	12.024	1789	1794	1799	rBV	296360	379530	12.54%	1.485%
80	12.091	1799	1805	1809	rVV	531391	663392	21.92%	2.596%
81	12.128	1809	1811	1813	rVV	47807	54328	1.79%	0.213%
82	12.152	1813	1815	1818	rVB	37479	37926	1.25%	0.148%
83	12.250	1826	1831	1834	rBV	349780	494441	16.34%	1.935%
84	12.323	1838	1843	1850	rVV2	161436	250924	8.29%	0.982%
85	12.469	1863	1867	1873	rVV2	55684	86135	2.85%	0.337%
86	12.536	1873	1878	1880	rVV	70118	94487	3.12%	0.370%
87	12.560	1880	1882	1887	rVV	56507	62720	2.07%	0.245%
88	12.615	1887	1891	1894	rVV	99587	118726	3.92%	0.465%
89	12.701	1901	1905	1914	rVB2	62121	119144	3.94%	0.466%
90	12.926	1935	1942	1945	rBV	38888	49998	1.65%	0.196%
91	12.963	1945	1948	1954	rVB	50813	62691	2.07%	0.245%
92	13.170	1973	1982	1986	rBV2	25105	36550	1.21%	0.143%
93	13.298	1998	2003	2009	rVB2	51096	72406	2.39%	0.283%

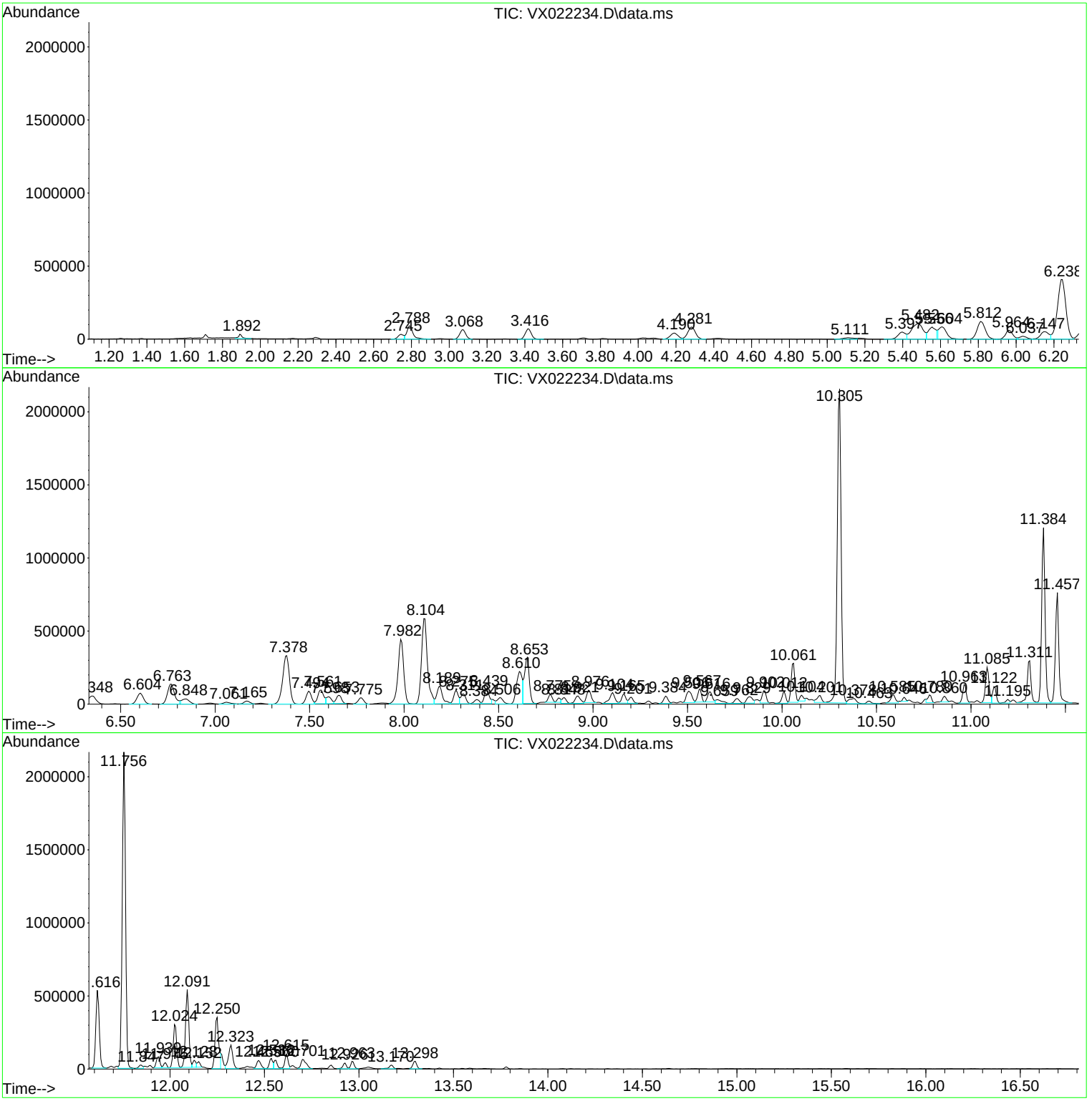
Sum of corrected areas: 25554705

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

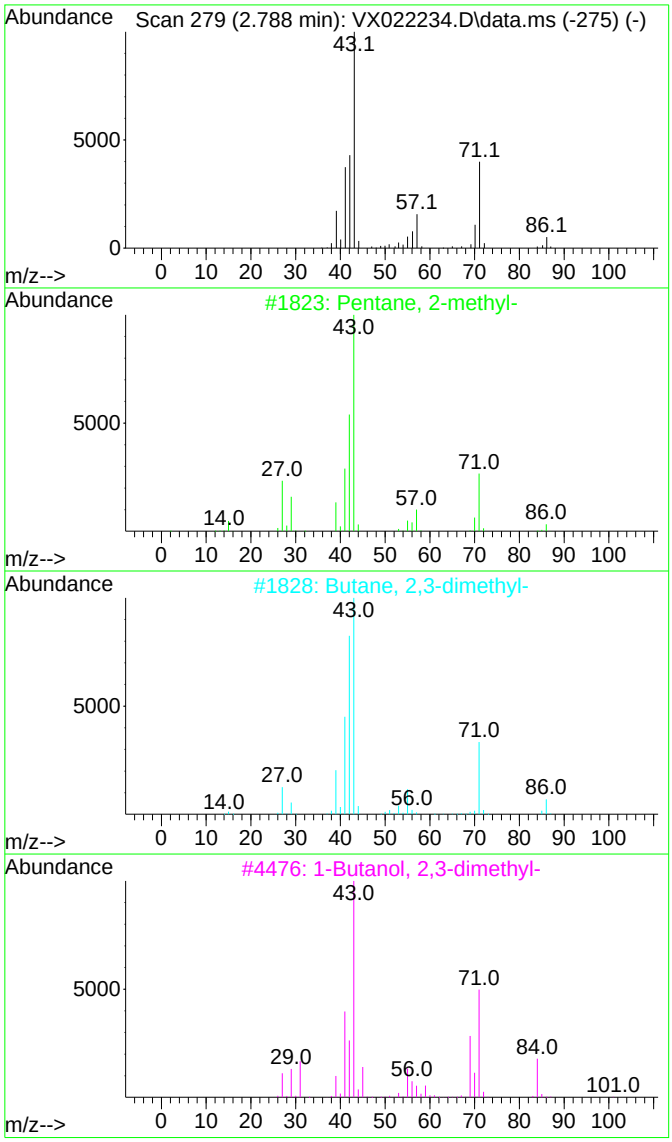
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

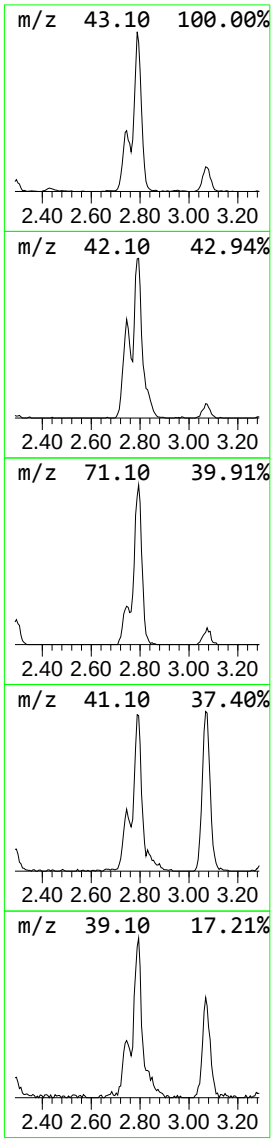
****

Peak Number 1 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.788	45.23 ug/l	202855	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	43
5	Pentane	72	C5H12	000109-66-0	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

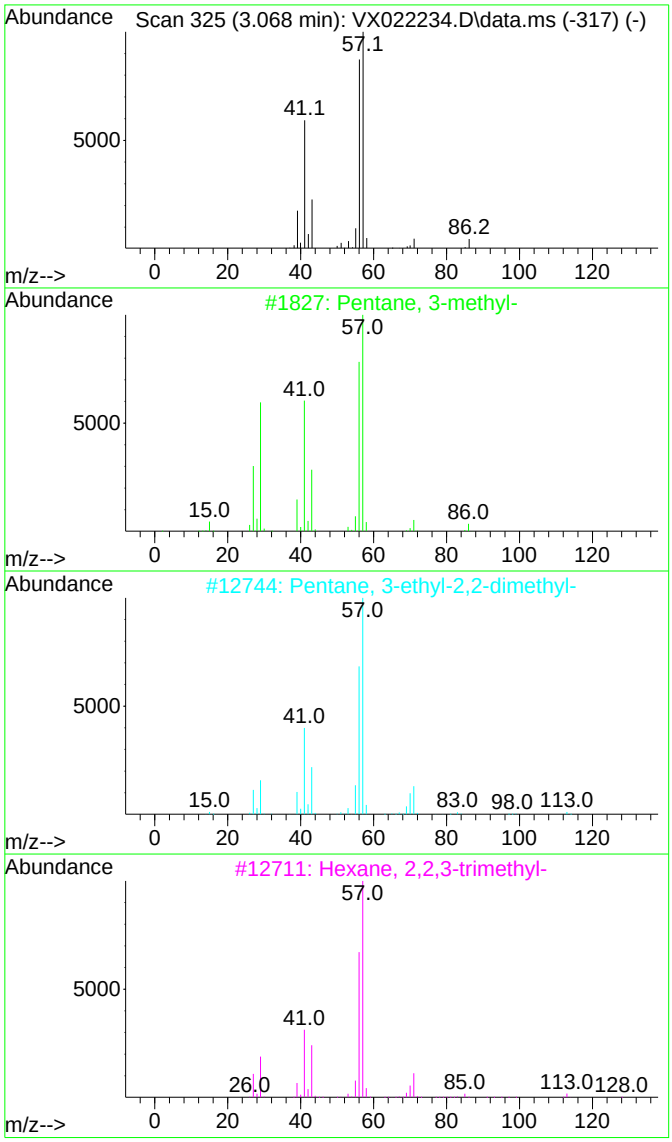
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

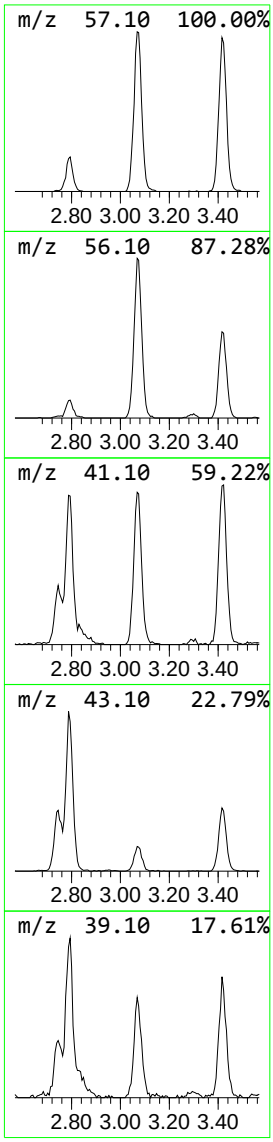
****

Peak Number 2 Pentane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.068	32.13 ug/l	144099	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

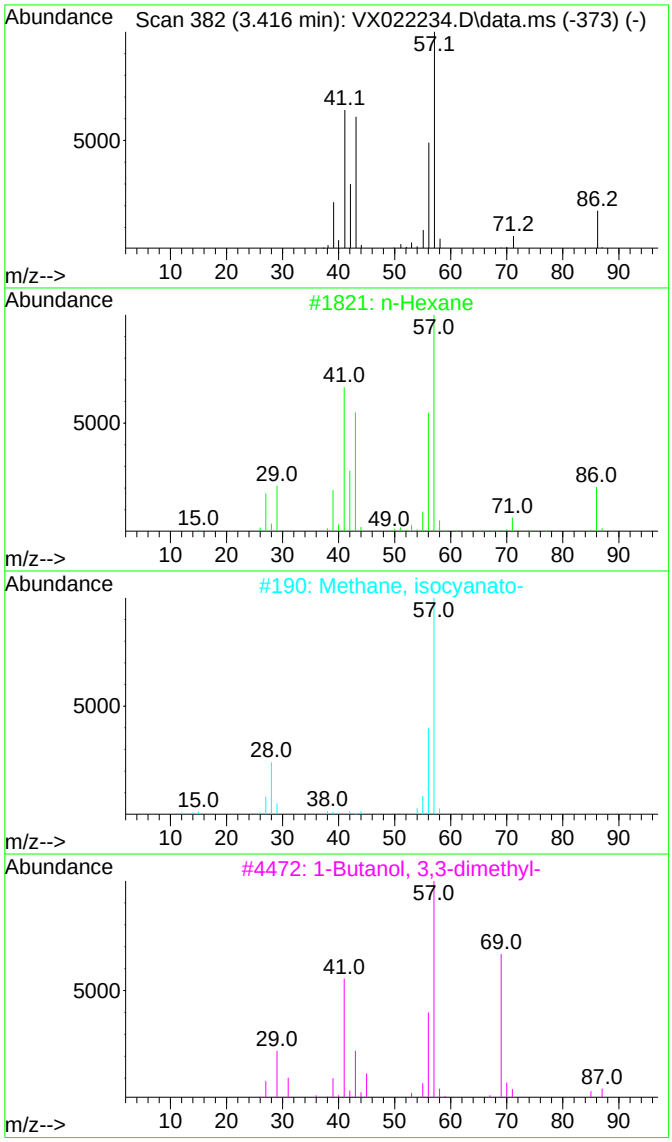
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

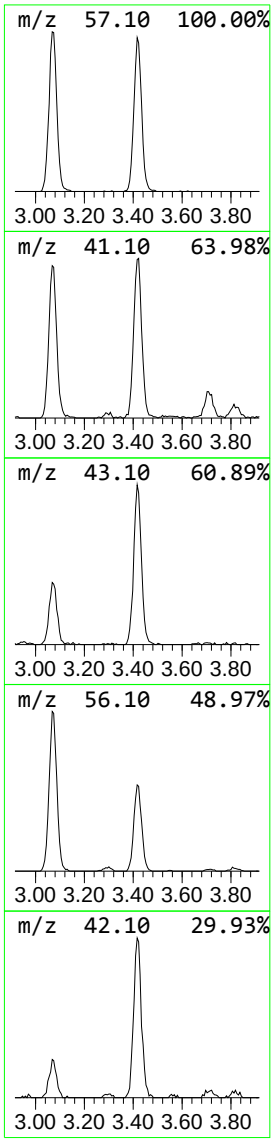
****

Peak Number 3 n-Hexane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	35.07 ug/l	157291	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	91
2	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
3	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	36
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	36
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

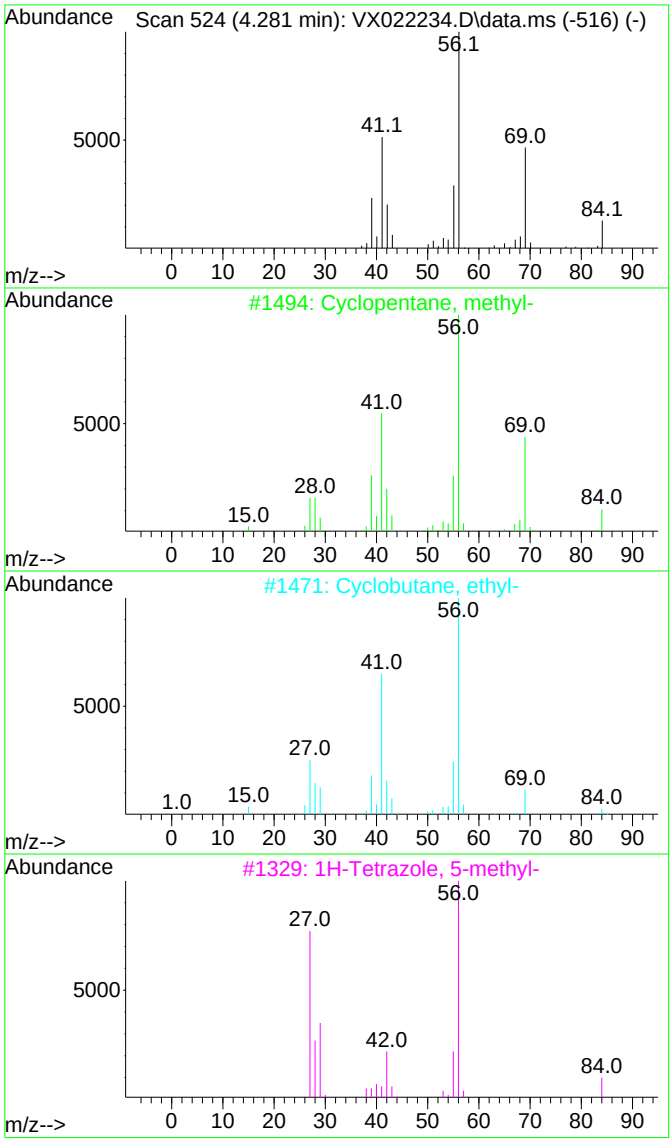
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

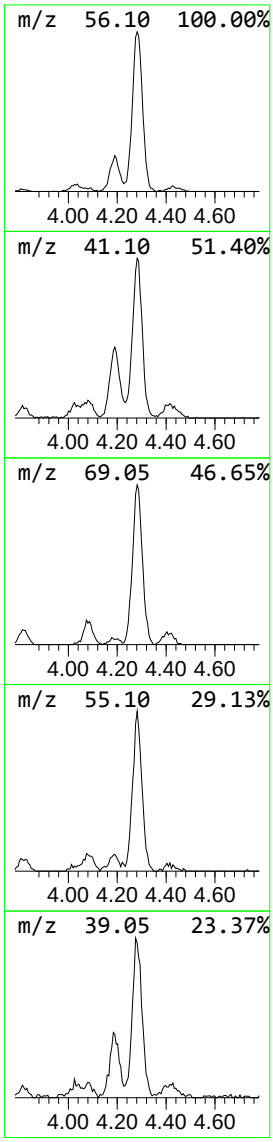
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	52.07 ug/l	233513	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	35
5	1-Hexene	84	C6H12	000592-41-6	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

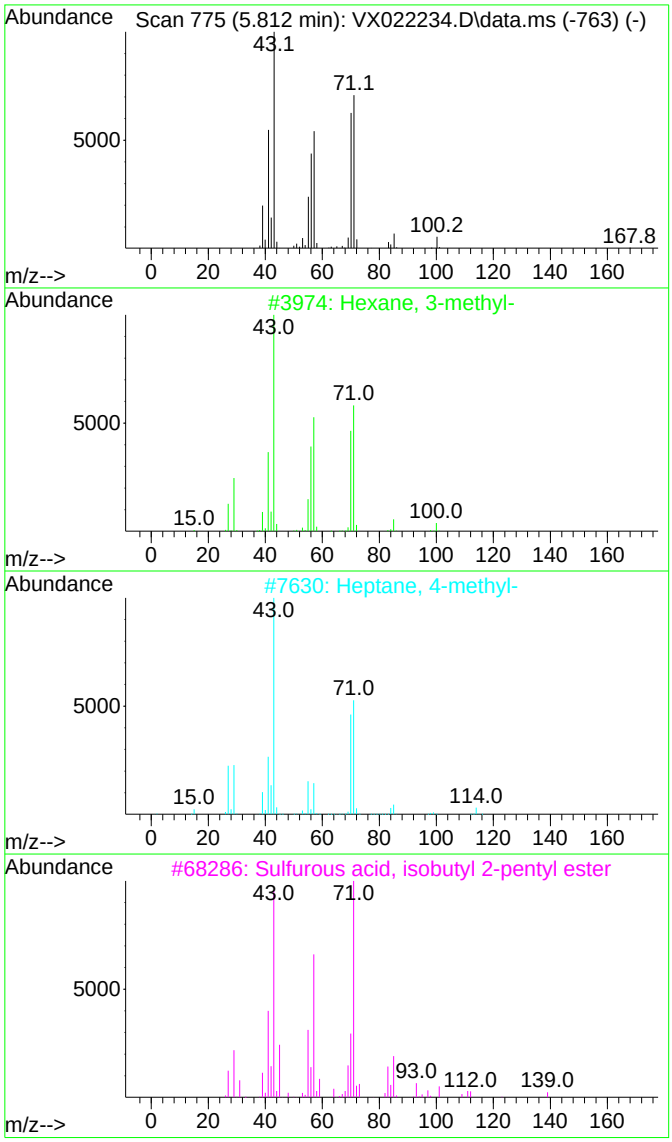
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

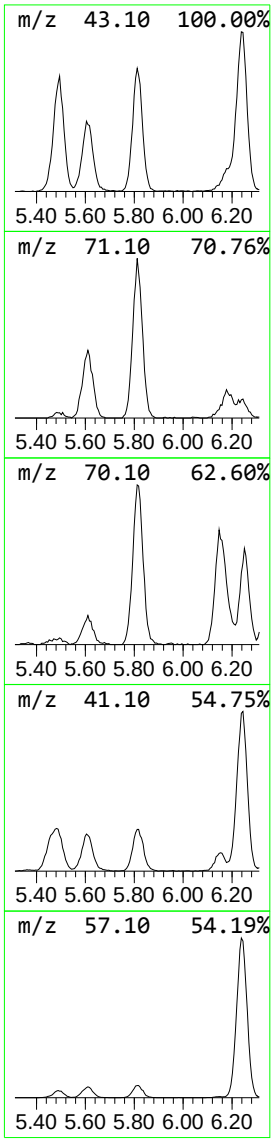
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	82.03 ug/l	367891	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
3	Sulfurous acid, isobutyl 2-penty...	208	C9H20O3S	1000309-15-2	53
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

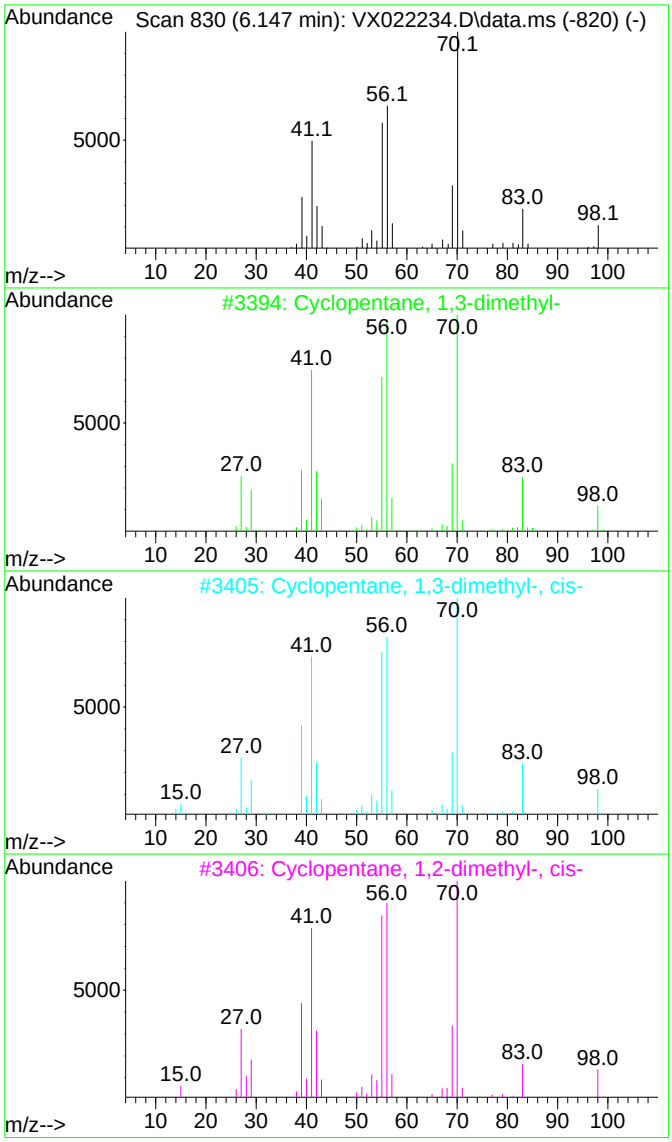
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

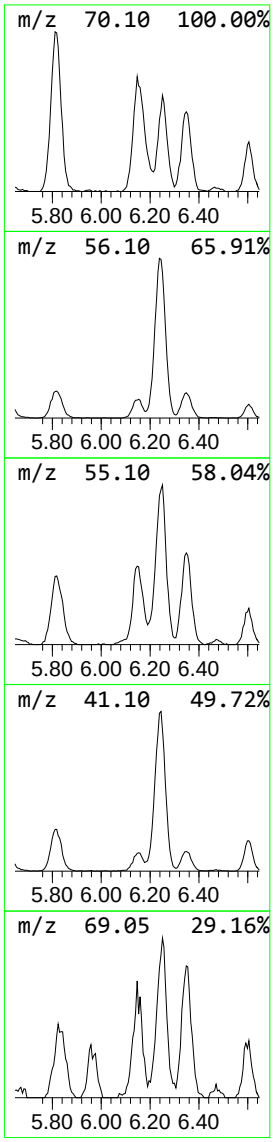
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, 1,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.147	36.85 ug/l	165278	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	95
2	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	76
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	76
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	68
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

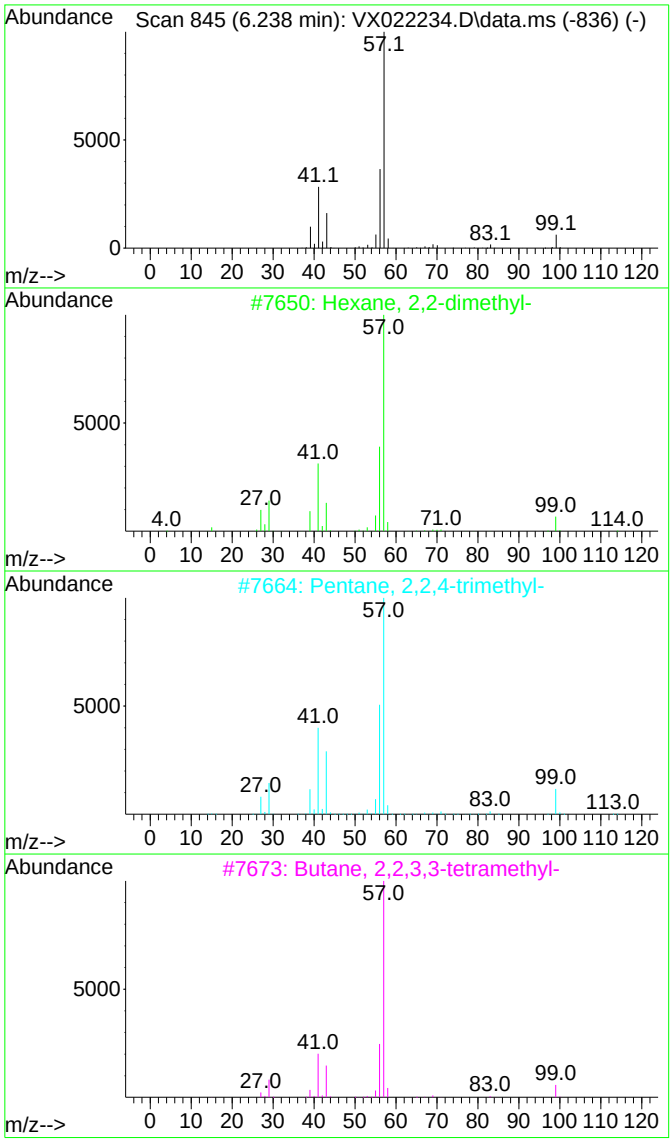
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

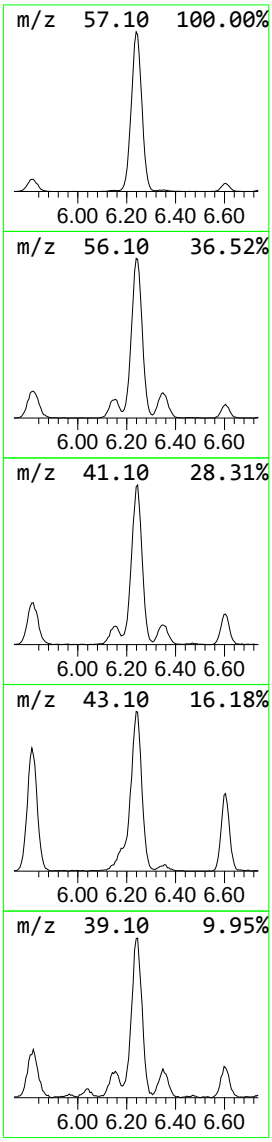
****

Peak Number 7 Hexane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.238	176.20 ug/l	1259330	1,4-Difluorobenzene	6.763

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

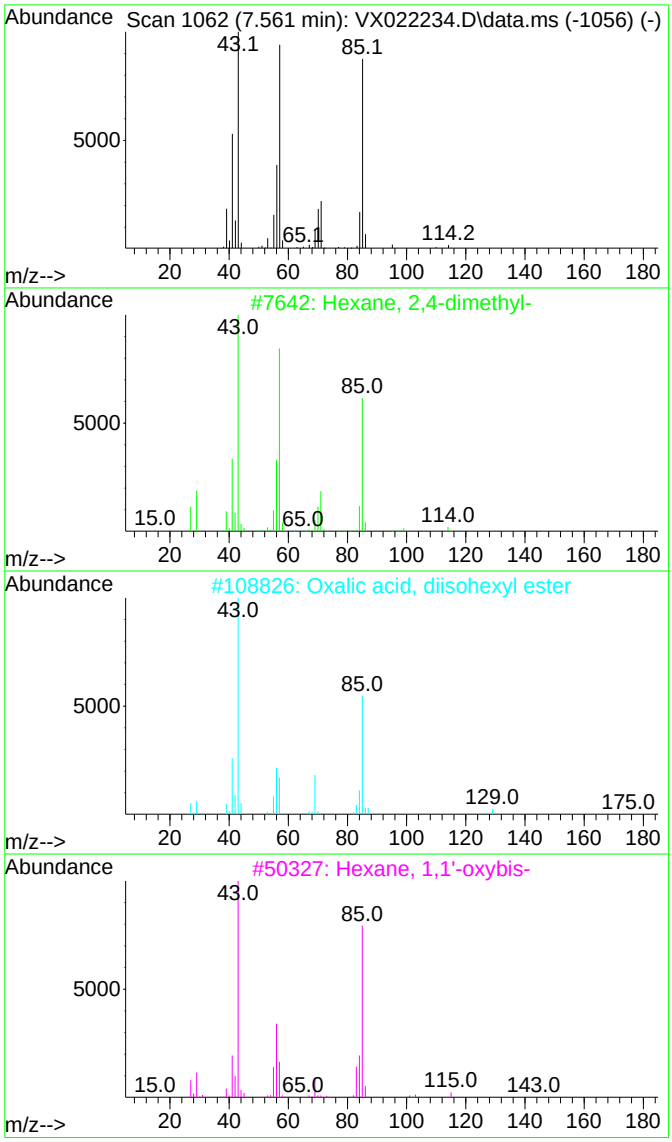
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

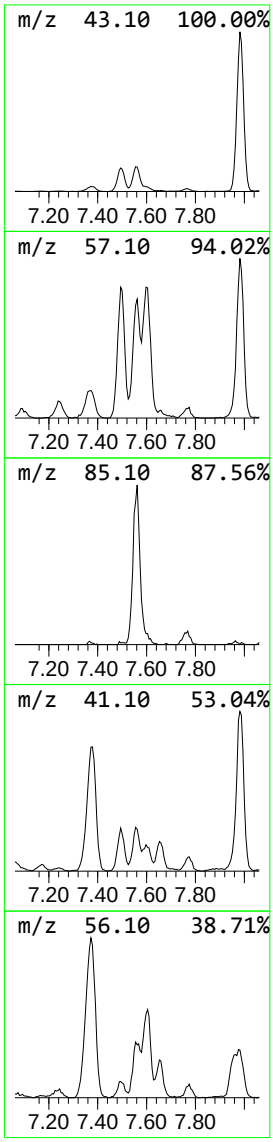
****

Peak Number 8 Hexane, 2,4-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.561	28.93 ug/l	206764	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	74
2	Oxalic acid, diisohexyl ester	258	C14H26O4	1000309-32-9	64
3	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	64
4	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	59
5	Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

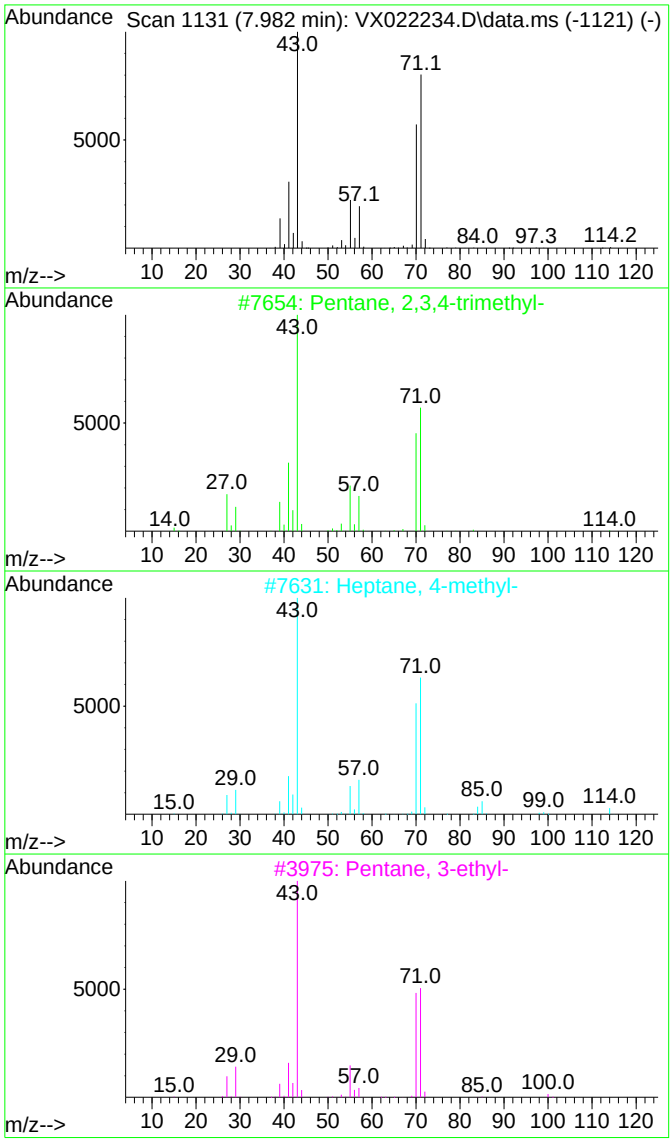
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

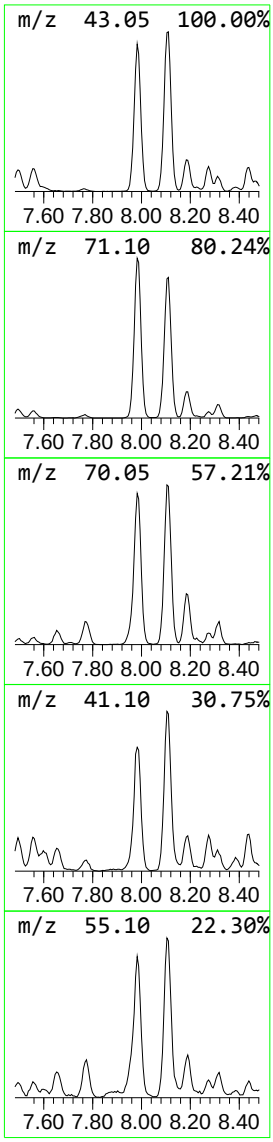
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	129.11 ug/l	922747	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

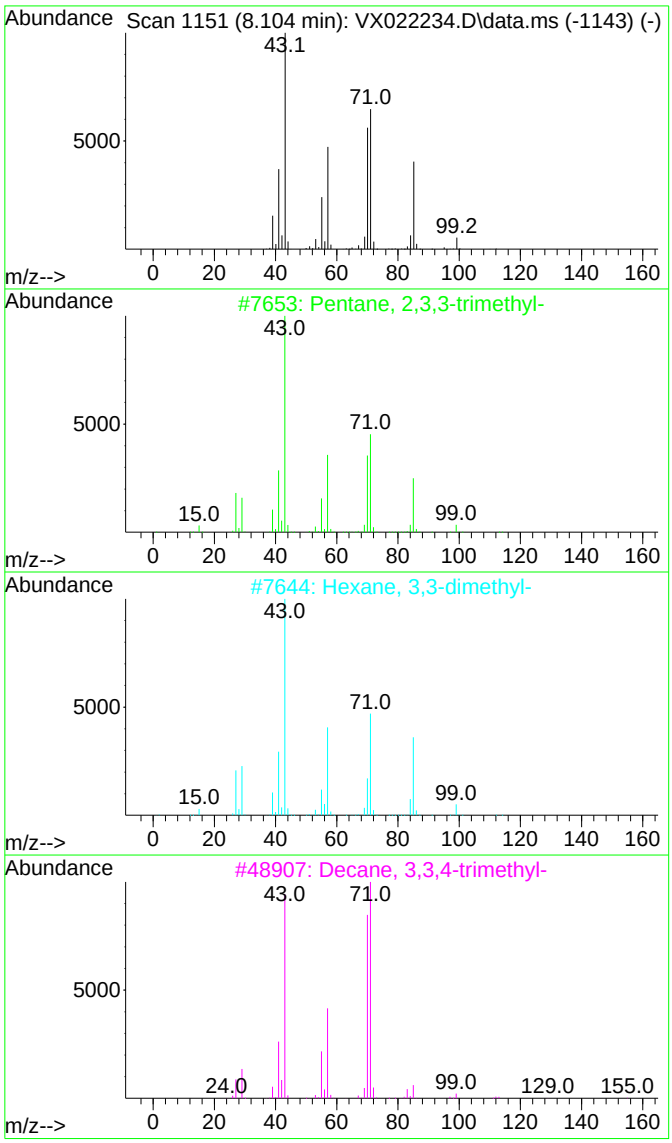
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

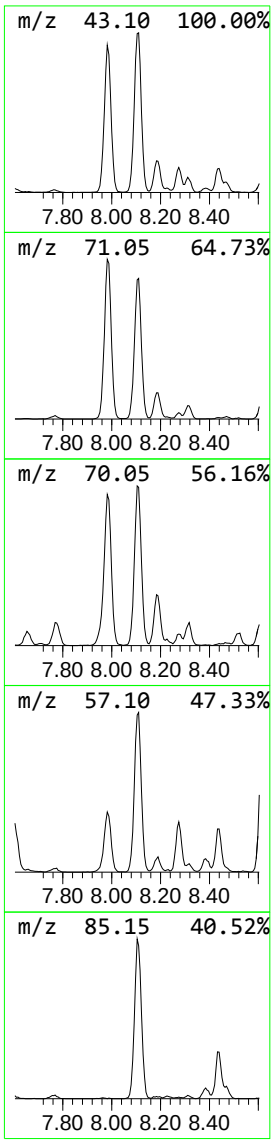
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	178.58 ug/l	1276290	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

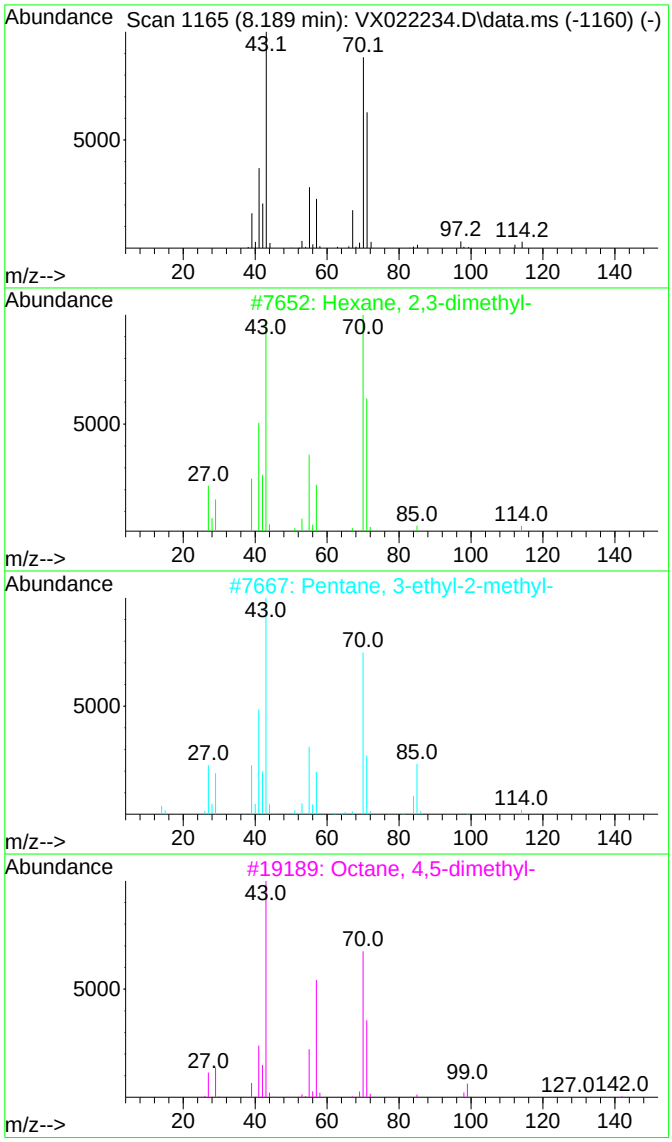
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

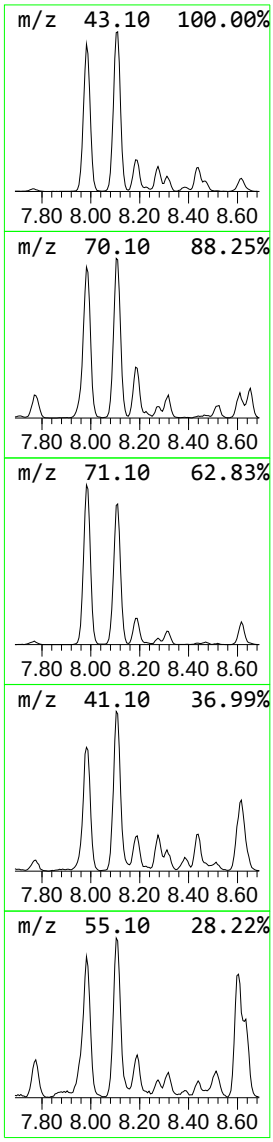
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Hexane, 2,3-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.189	35.59 ug/l	254392	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	86
2	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	72
3	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

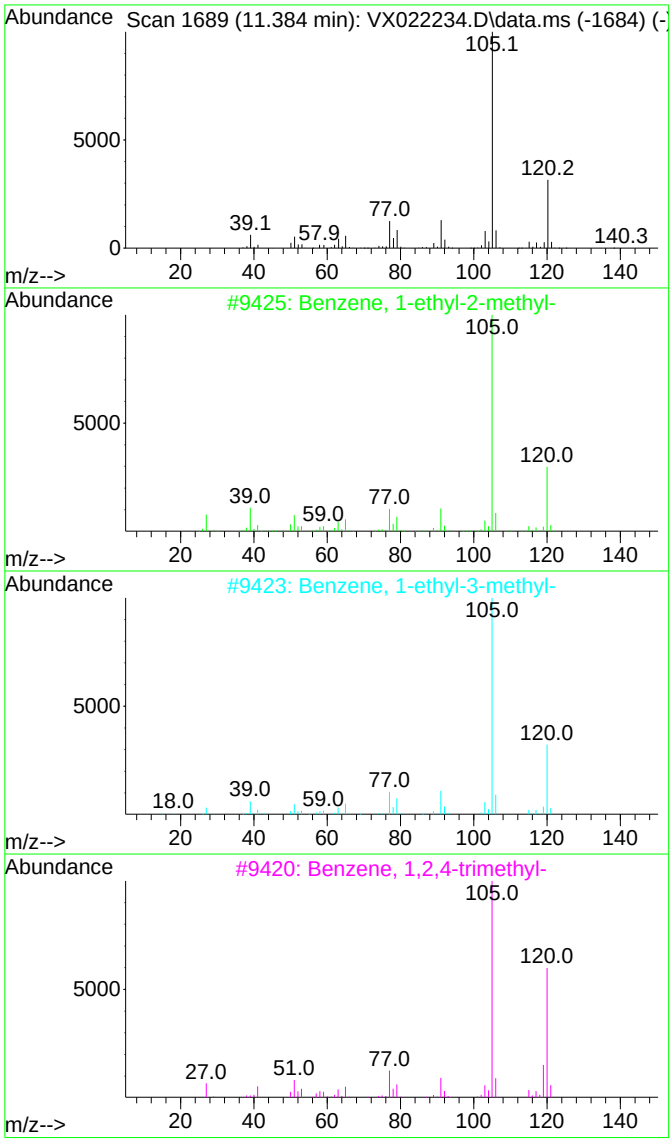
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

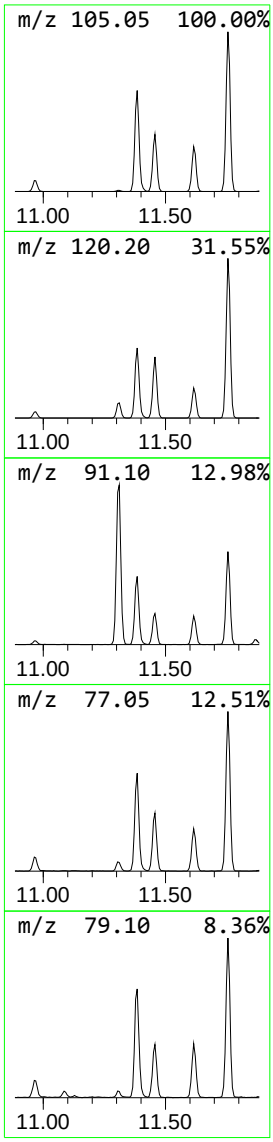
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	195.03 ug/l	1480380	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

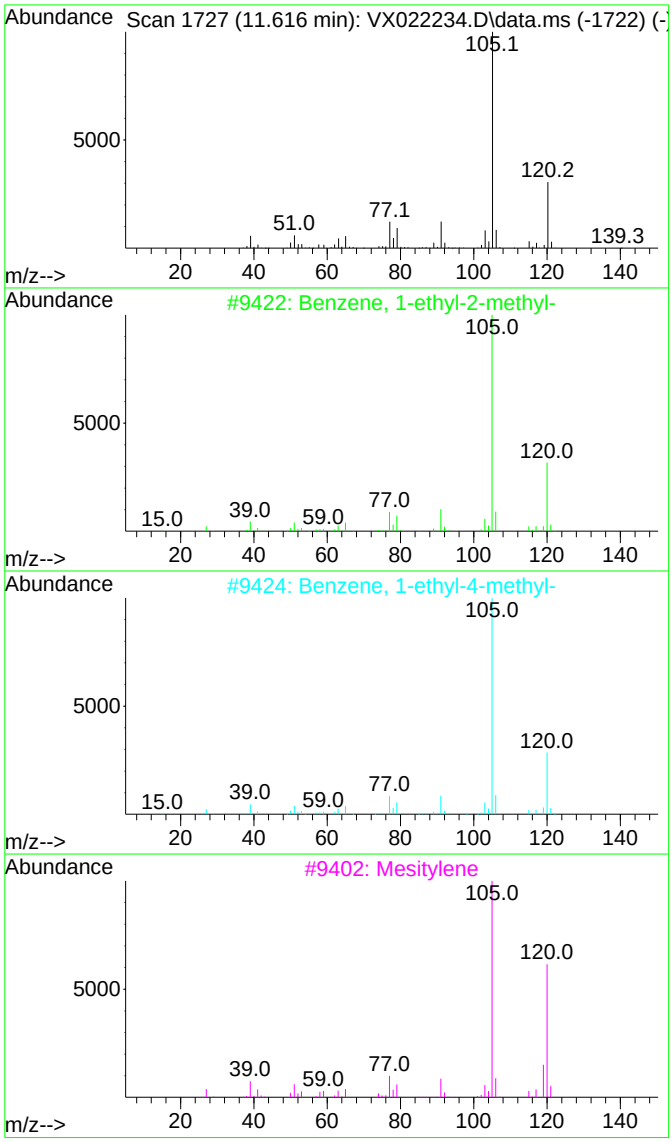
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

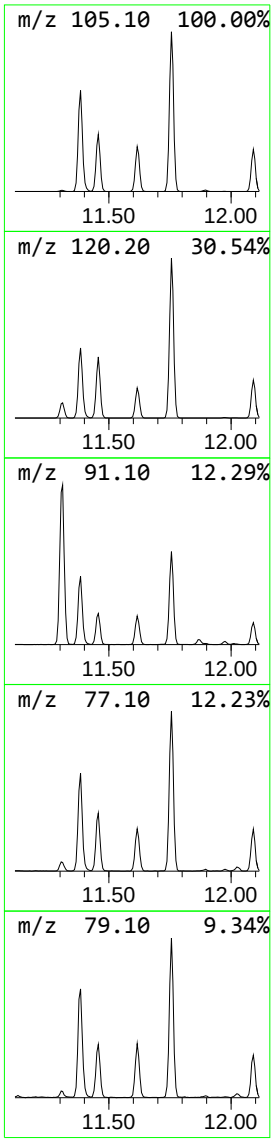
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	86.69 ug/l	658044	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

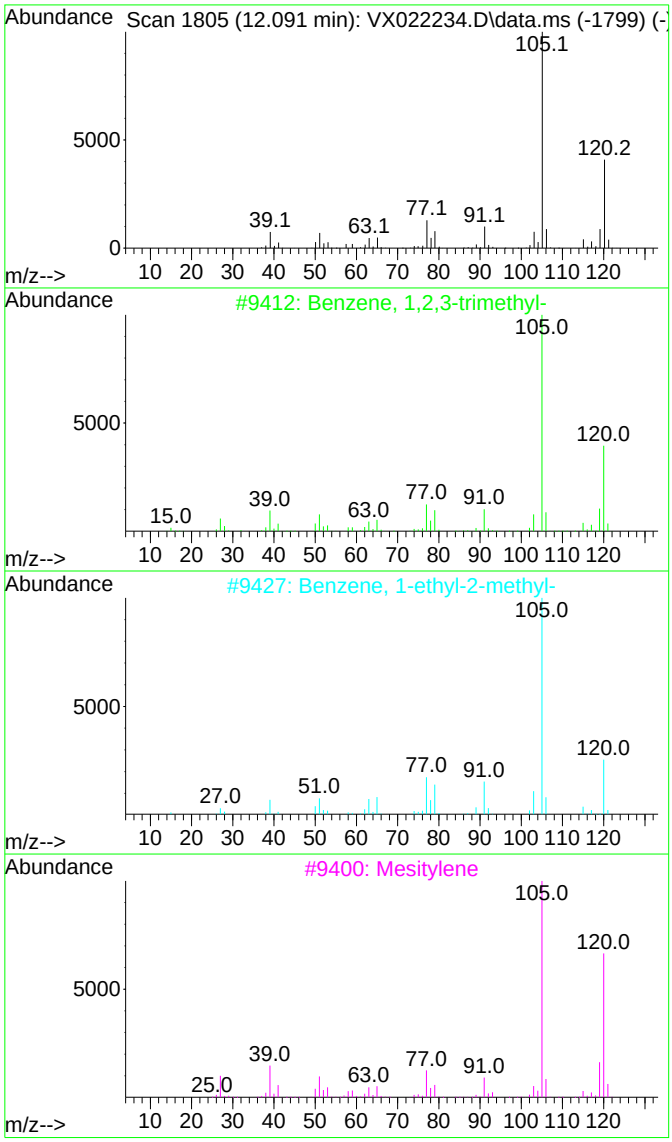
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

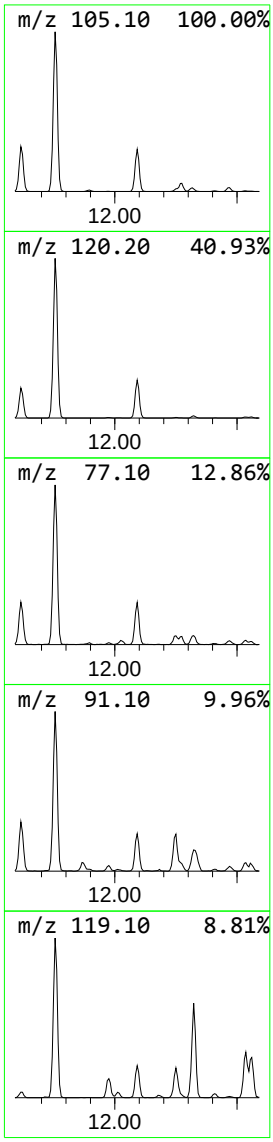
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	87.40 ug/l	663392	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GHOST-2D

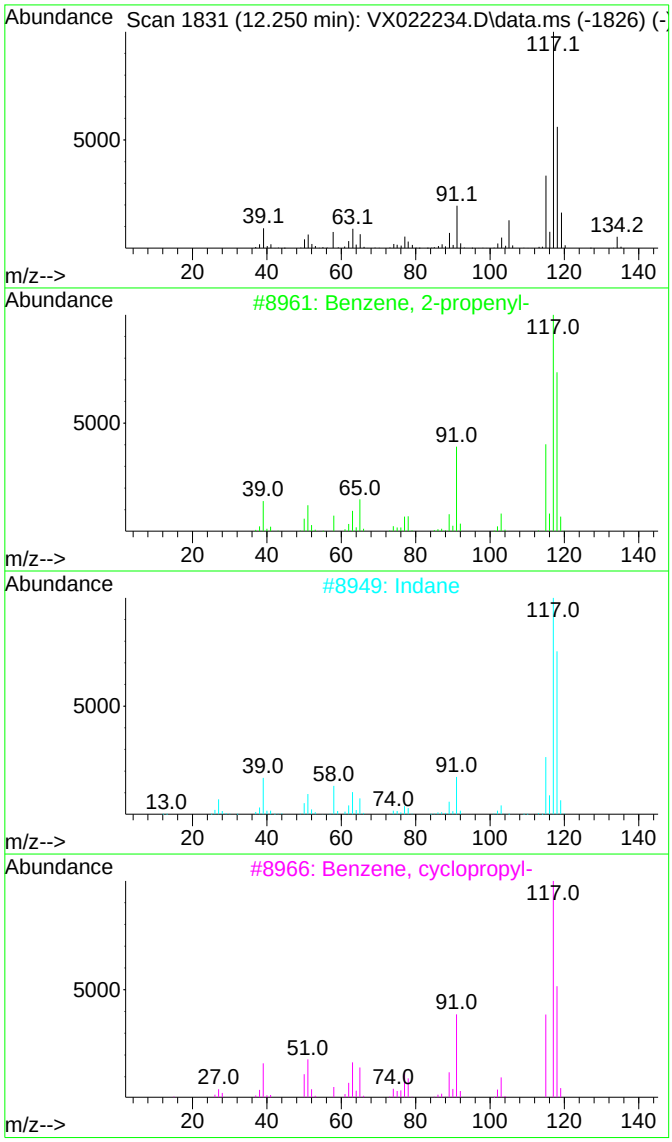
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

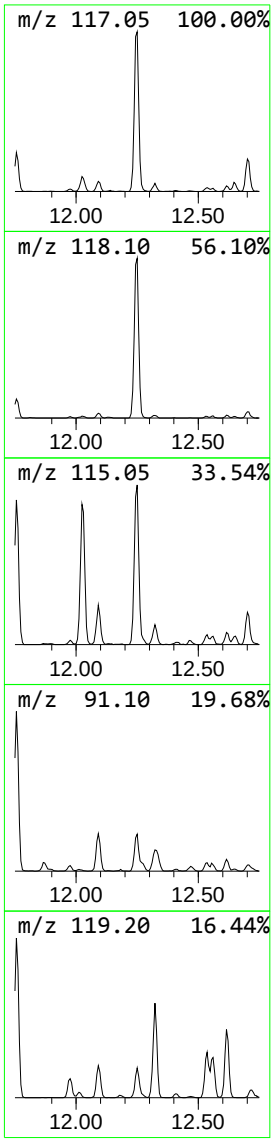
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.249	65.14 ug/l	494441	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2	Indane	118	C9H10	000496-11-7	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052821\
Data File : VX022234.D
Acq On : 27 May 2021 15:53
Operator : JC/MD
Sample : M2535-02
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GHOST-2D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.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
Pentane, 2-methyl-	2.788	45.2	ug/l	202855	1	5.556	224249	50.0
Pentane, 3-methyl-	3.068	32.1	ug/l	144099	1	5.556	224249	50.0
n-Hexane	3.416	35.1	ug/l	157291	1	5.556	224249	50.0
Cyclopentane, m...	4.281	52.1	ug/l	233513	1	5.556	224249	50.0
Hexane, 3-methyl-	5.812	82.0	ug/l	367891	1	5.556	224249	50.0
Cyclopentane, 1...	6.147	36.9	ug/l	165278	1	5.556	224249	50.0
Hexane, 2,2-dim...	6.238	176.2	ug/l	1259330	2	6.763	357354	50.0
Hexane, 2,4-dim...	7.561	28.9	ug/l	206764	2	6.763	357354	50.0
Pentane, 2,3,4-...	7.982	129.1	ug/l	922747	2	6.763	357354	50.0
Pentane, 2,3,3-...	8.104	178.6	ug/l	1276290	2	6.763	357354	50.0
Hexane, 2,3-dim...	8.189	35.6	ug/l	254392	2	6.763	357354	50.0
Benzene, 1-ethy...	11.384	195.0	ug/l	1480380	4	12.030	379530	50.0
Benzene, 1-ethy...	11.616	86.7	ug/l	658044	4	12.030	379530	50.0
Benzene, 1,2,3-...	12.091	87.4	ug/l	663392	4	12.030	379530	50.0
Benzene, 2-prop...	12.249	65.1	ug/l	494441	4	12.030	379530	50.0