LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SPILL-COMP-31277-AUD-1077

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_N\methods\82N062821W.M
Title : SW846 8260

Signal : TIC: VN067577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.413	144	158	179	rBV2	64350	137552	3.41%	0.388%
2	6.474	1649	1672	1697	rBV5	11144	40505	1.00%	0.114%
3	8.018	2227	2248	2257	rBV2	233423	564928	13.99%	1.593%
4	8.080	2260	2271	2290	rVV	433002	1034075	25.61%	2.915%
5	8.158	2292	2300	2324	rVB6	23337	56861	1.41%	0.160%
6	8.284	2329	2347	2368	rBV2	92508	213398	5.29%	0.602%
7	8.434	2382	2403	2428	rBV	276450	626462	15.52%	1.766%
8	8.820	2528	2547	2567	rBV2	119233	246689	6.11%	0.696%
9	8.965	2583	2601	2634	rVB	643063	1349156	33.41%	3.804%
10	9.453	2757	2783	2795	rBV4	41180	99123	2.45%	0.279%
11	9.877	2920	2941	2960	rBV4	21698	45762	1.13%	0.129%
12	10.014	2975	2992	3004	rBV3	28158	57225	1.42%	0.161%
13	10.076	3005	3015	3040	rVB4	27705	67213	1.66%	0.189%
14	10.215	3046	3067	3090	rBV2	27121	63144	1.56%	0.178%
15	10.443	3134	3152	3163	rVV	1132578	2124184	52.61%	5.989%
16	10.507	3163	3176	3205	rVV	2107770	4037718	100.00%	11.384%
17	10.623	3207	3219	3237	rVB2	76121	147507	3.65%	0.416%
18	10.877	3300	3314	3336	rVV10	20067	54091	1.34%	0.153%
19	11.052	3367	3379	3391	rBV2	24645	43836	1.09%	0.124%
20	11.154	3406	3417	3434	rBV2	30301	61886	1.53%	0.174%
21	11.293	3461	3469	3479	rVB	34087	50495	1.25%	0.142%
22	11.347	3479	3489	3501	rVB2	45113	76244	1.89%	0.215%
23	11.457	3520	3530	3537	rBV6	26391	42286	1.05%	0.119%
24	11.529	3538	3557	3582	rVB7	175745	451281	11.18%	1.272%
25	11.628	3582	3594	3616	rVB	137889	234093	5.80%	0.660%
26	11.749	3620	3639	3659	rBV	1061576	1931571	47.84%	5.446%
27	11.848	3663	3676	3695	rVB	197727	350309	8.68%	0.988%
28	11.956	3696	3716	3738	rBV3	1540622	3050217	75.54%	8.600%
29	12.178	3787	3799	3811	rVB6	48273	93135	2.31%	0.263%
30	12.283	3812	3838	3854	rBV	515932	1205197	29.85%	3.398%
31	12.369	3863	3870	3880	rVB	95852	144747	3.58%	0.408%
32	12.452	3881	3901	3907	rBV10	67499	169527	4.20%	0.478%
33	12.583	3940	3950	3958	rBV4	56422	113022	2.80%	0.319%
34	12.733	3995	4006	4030	rVB	909751	1734774	42.96%	4.891%
35	12.921	4065	4076	4087	rVB	185845	315456	7.81%	0.889%
36	12.986	4087	4100	4108	rBV	745421	1293854	32.04%	3.648%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SPILL-COMP-31277-AUD-1077

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_N\methods\82N062821W.M
Title : SW846 8260

37	13.055	4117	4126	4140	rVB4	906516	1711500	42.39%	4.825%
38	13.109	4142	4146	4160	rVB4	63668	90842	2.25%	0.256%
39	13.224	4172	4189	4204	rBV	297649	587091	14.54%	1.655%
40	13.286	4206	4212	4228	rVB5	51921	87454	2.17%	0.247%
41	13.372	4230	4244	4258	rBV	1505666	2430332	60.19%	6.852%
42	13.565	4308	4316	4326	rVB4	112176	174635	4.33%	0.492%
43	13.610	4327	4333	4341	rVV5	41805	59368	1.47%	0.167%
44	13.677	4344	4358	4401	rVB2	1384726	3011377	74.58%	8.490%
45	13.844	4409	4420	4421	rBV3	77316	90837	2.25%	0.256%
46	13.873	4423	4431	4439	rVV3	329862	587910	14.56%	1.658%
47	13.911	4441	4445	4467	rVB3	258429	480222	11.89%	1.354%
48	13.997	4467	4477	4489	rBV4	157835	246711	6.11%	0.696%
49	14.072	4498	4505	4516	rVB	61984	87633	2.17%	0.247%
50	14.133	4518	4528	4533	rBV	119208	178268	4.42%	0.503%
51	14.219	4549	4560	4572	rVB	202131	320397	7.94%	0.903%
52	14.329	4590	4601	4613	rVB2	111121	188904	4.68%	0.533%
53	14.461	4640	4650	4660	rBV2	50208	89308	2.21%	0.252%
54	14.541	4674	4680	4688	rVV	66061	98319	2.44%	0.277%
55	14.581	4688	4695	4704	rVB	110211	150733	3.73%	0.425%
56	14.624	4704	4711	4715	rBV2	41921	52254	1.29%	0.147%
57	14.812	4772	4781	4787	rBV	77477	122516	3.03%	0.345%
58	14.849	4788	4795	4807	rVB4	152135	235471	5.83%	0.664%
59	14.930	4809	4825	4836	rBV4	137790	353242	8.75%	0.996%
60	15.088	4877	4884	4899	rVB5	27466	51070	1.26%	0.144%
61	15.198	4918	4925	4935	rVB6	35605	49762	1.23%	0.140%
62	15.469	5016	5026	5033	rBV5	82474	147794	3.66%	0.417%
63	15.705	5104	5114	5134	rVB2	260612	488915	12.11%	1.378%
64	16.327	5332	5346	5364	rBV4	421717	968413	23.98%	2.730%

Sum of corrected areas: 35468801

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Data File : VN067577.D
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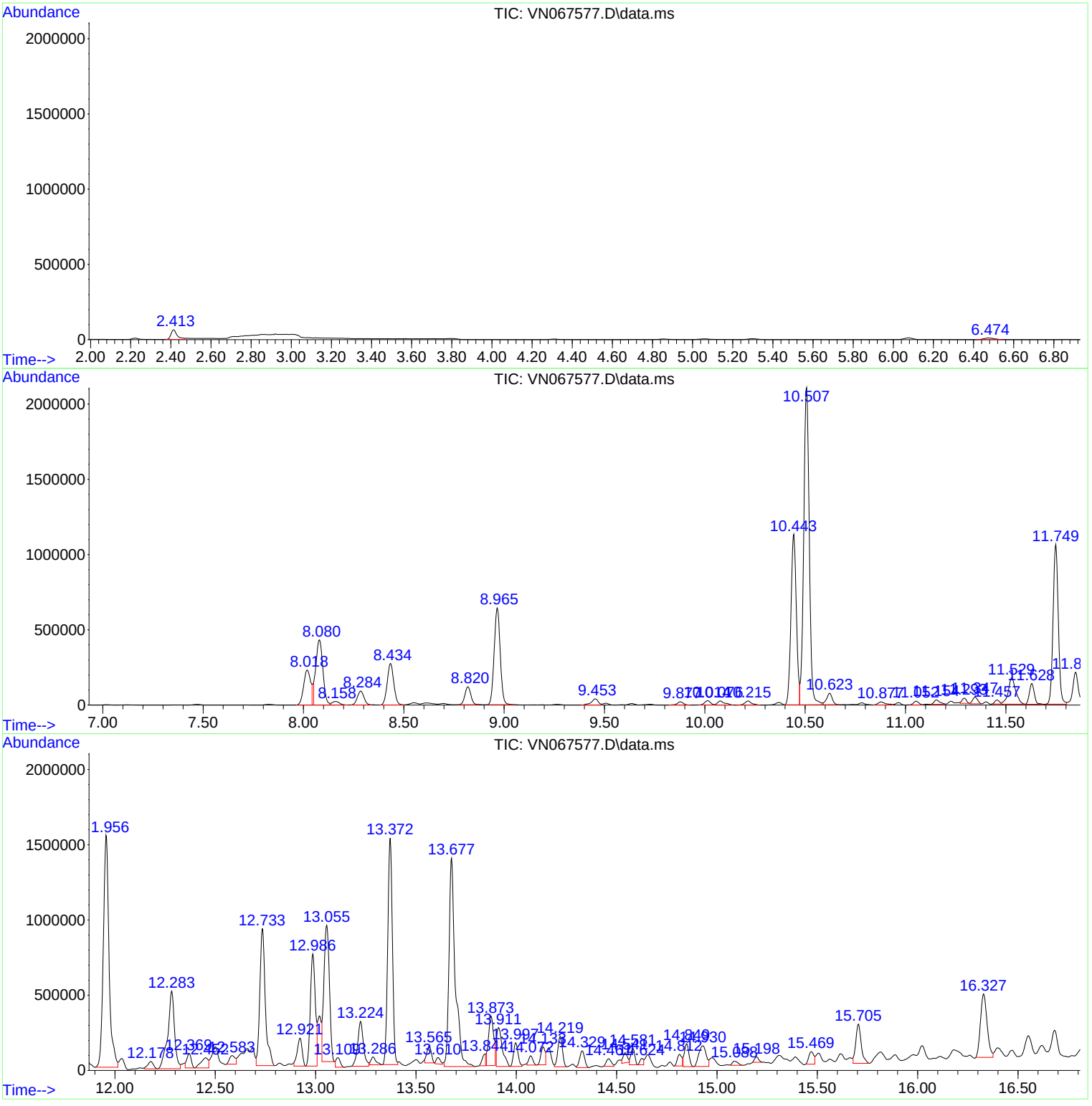
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
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Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

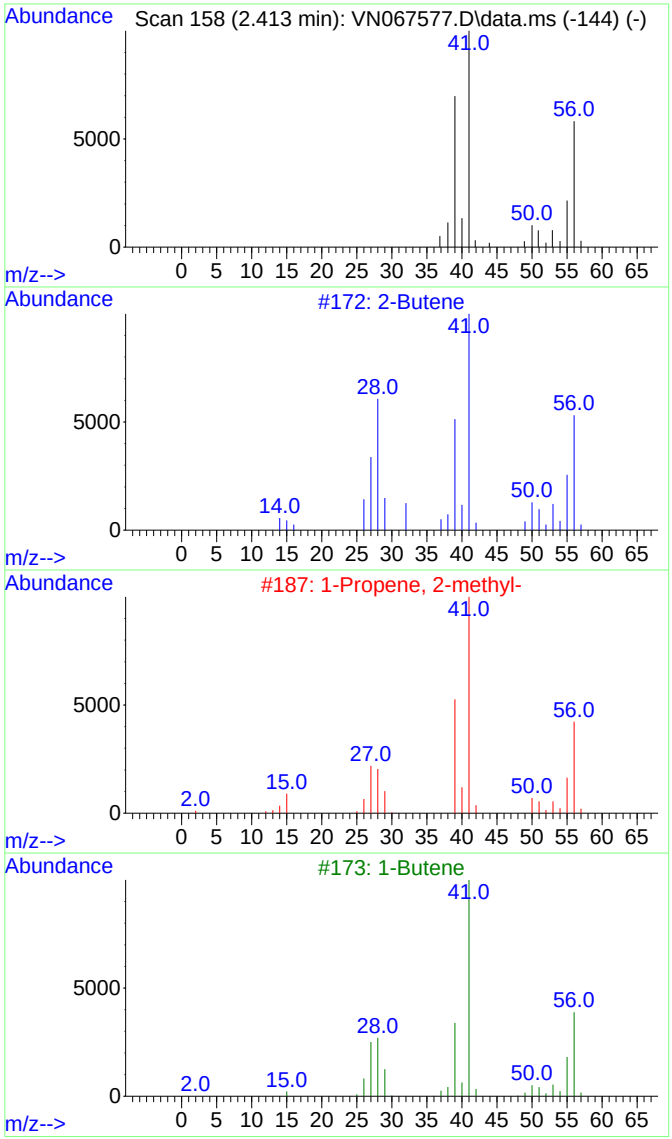
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

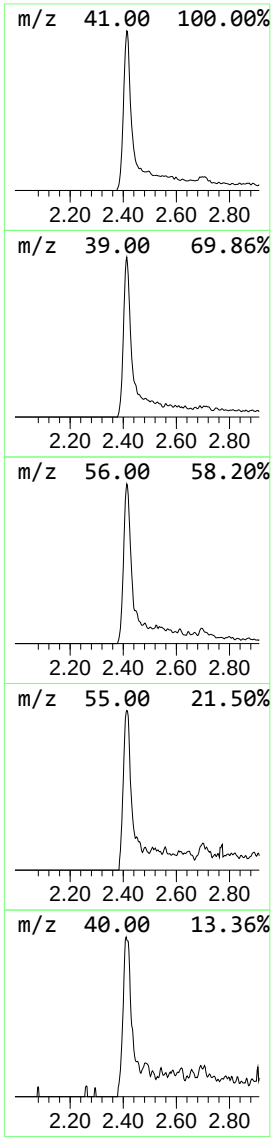
****

Peak Number 1 2-Butene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.413	6.65 ug/l	137552	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene	56	C4H8	000107-01-7	72
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	59
3	1-Butene	56	C4H8	000106-98-9	49
4	2-Butene, (Z)-	56	C4H8	000590-18-1	46
5	Cyclobutane	56	C4H8	000287-23-0	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

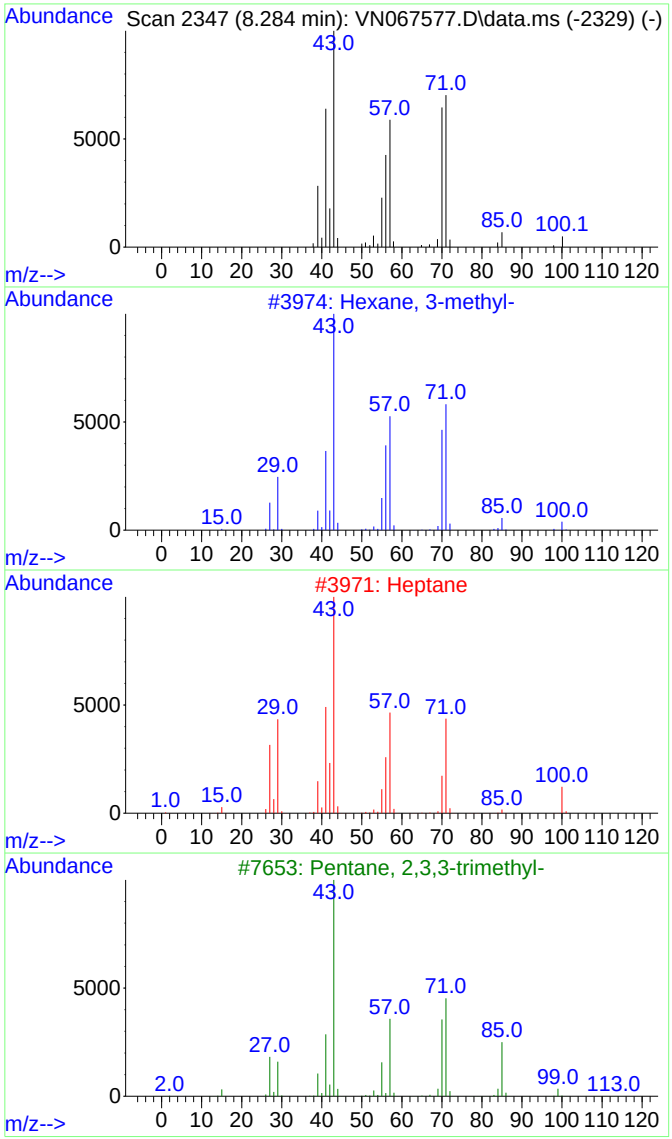
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

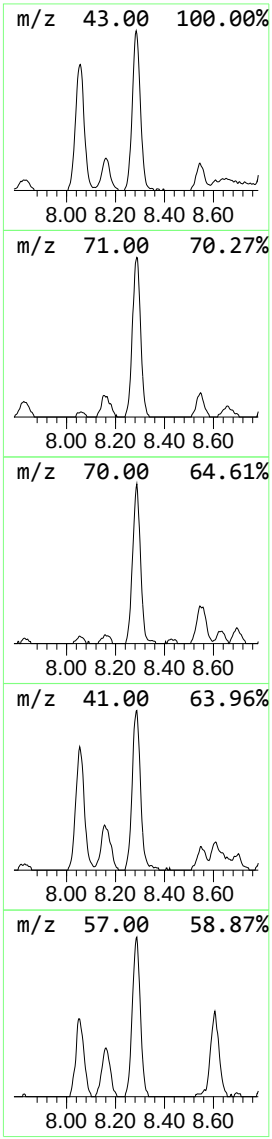
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	10.32 ug/l	213398	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

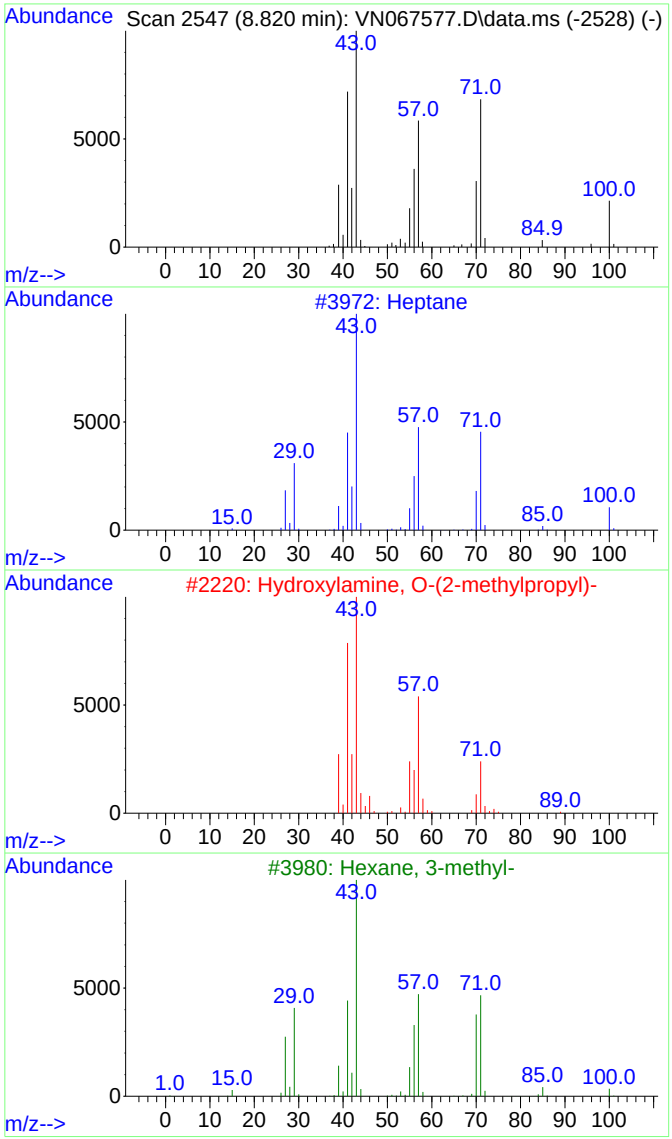
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

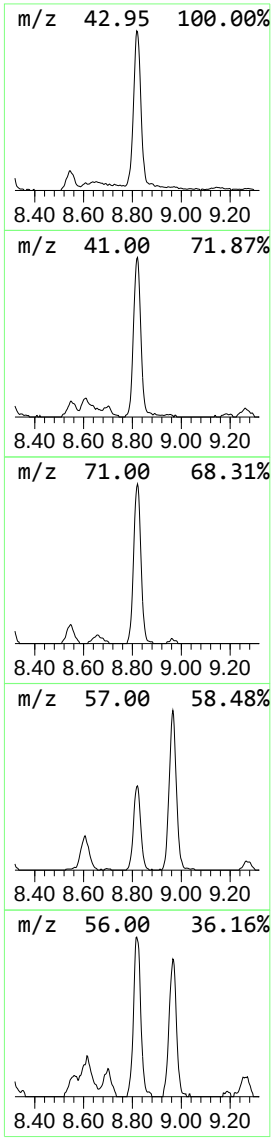
****

Peak Number 3 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.820	9.14 ug/l	246689	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	64
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
4	3-Hexanone	100	C6H12O	000589-38-8	43
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

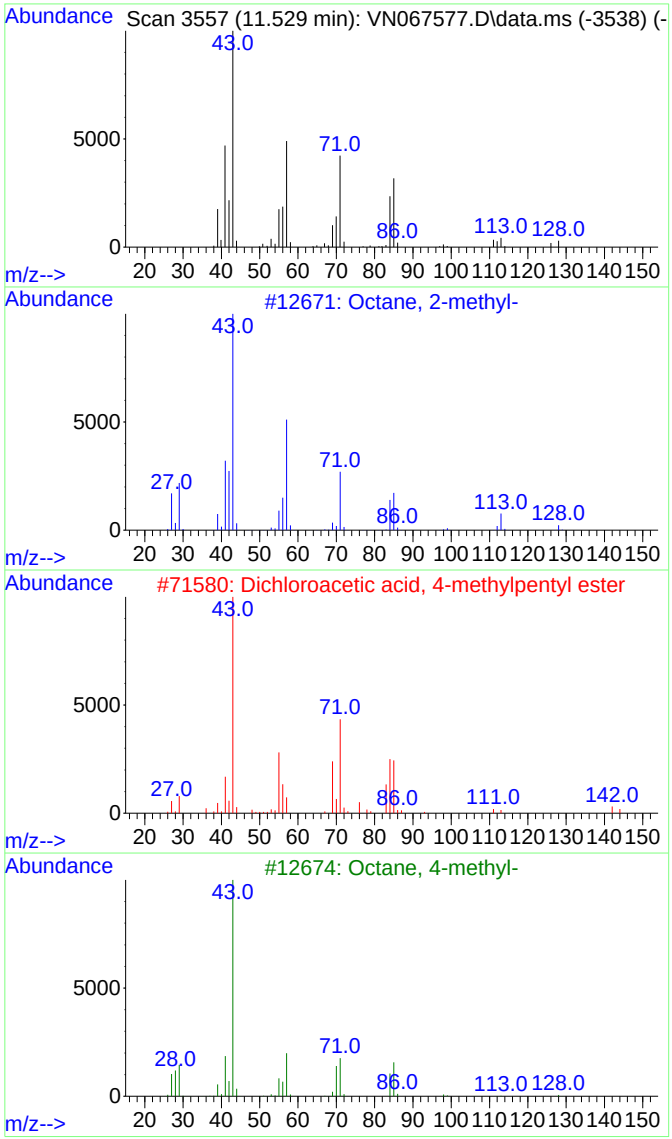
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

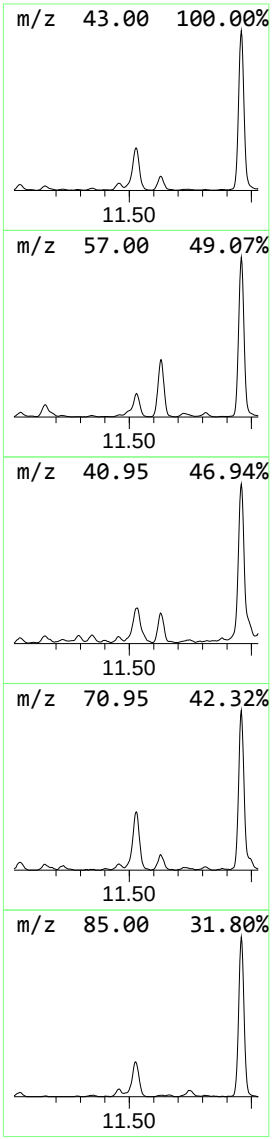
****

Peak Number 4 Octane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	11.68 ug/l	451281	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	74
2	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	53
3	Octane, 4-methyl-	128	C9H20	002216-34-4	53
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
5	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

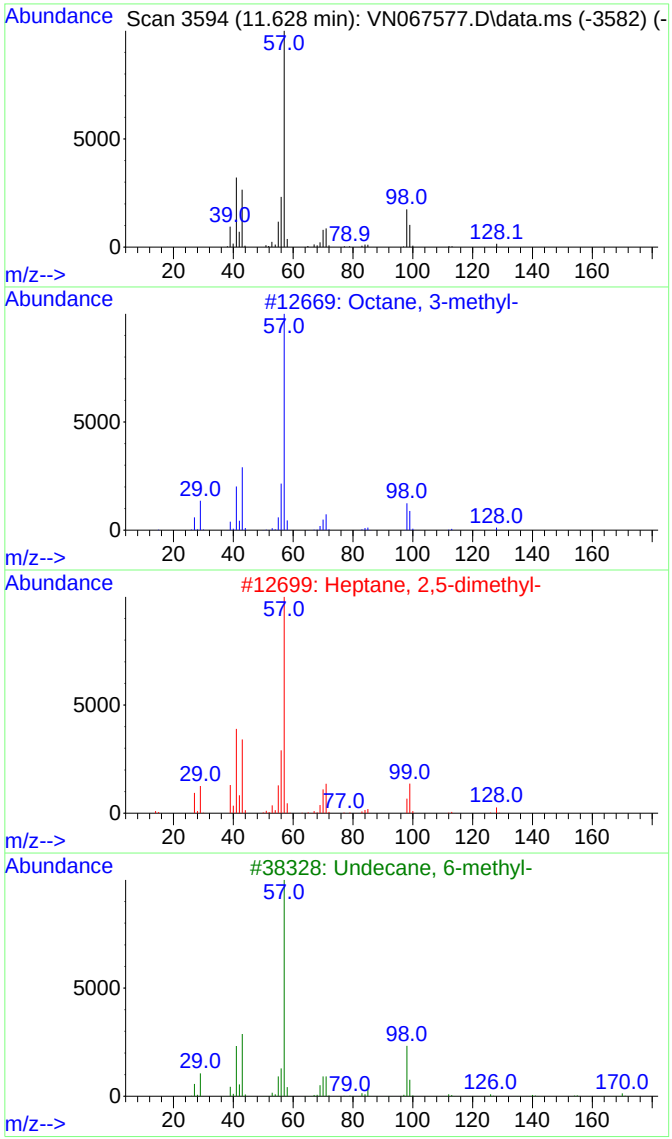
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

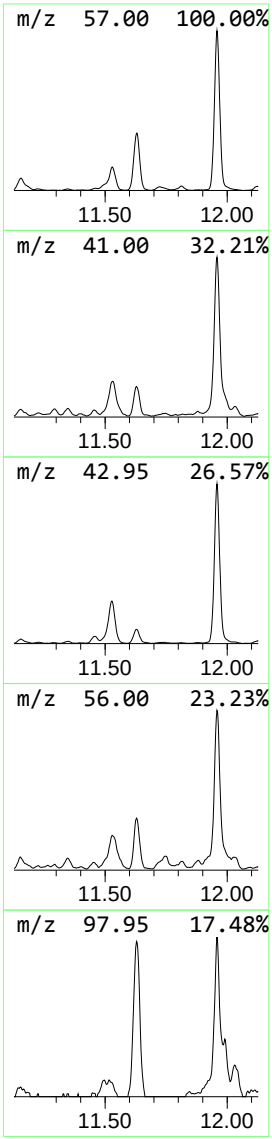
****

Peak Number 5 Octane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.628	6.06 ug/l	234093	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	81
3	Undecane, 6-methyl-	170	C12H26	017302-33-9	59
4	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	53
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	49





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Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

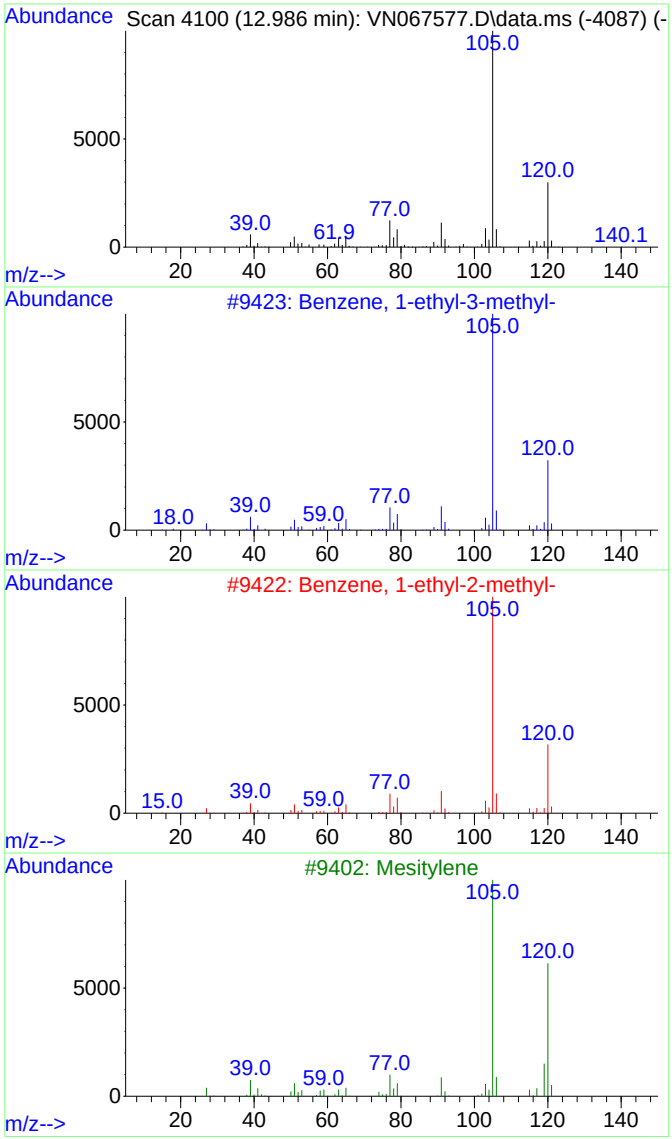
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

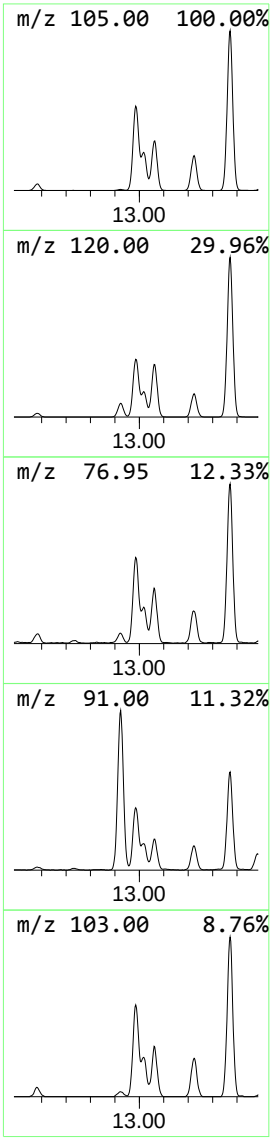
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	21.48 ug/l	1293850	1,4-Dichlorobenzene-d4	13.678

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

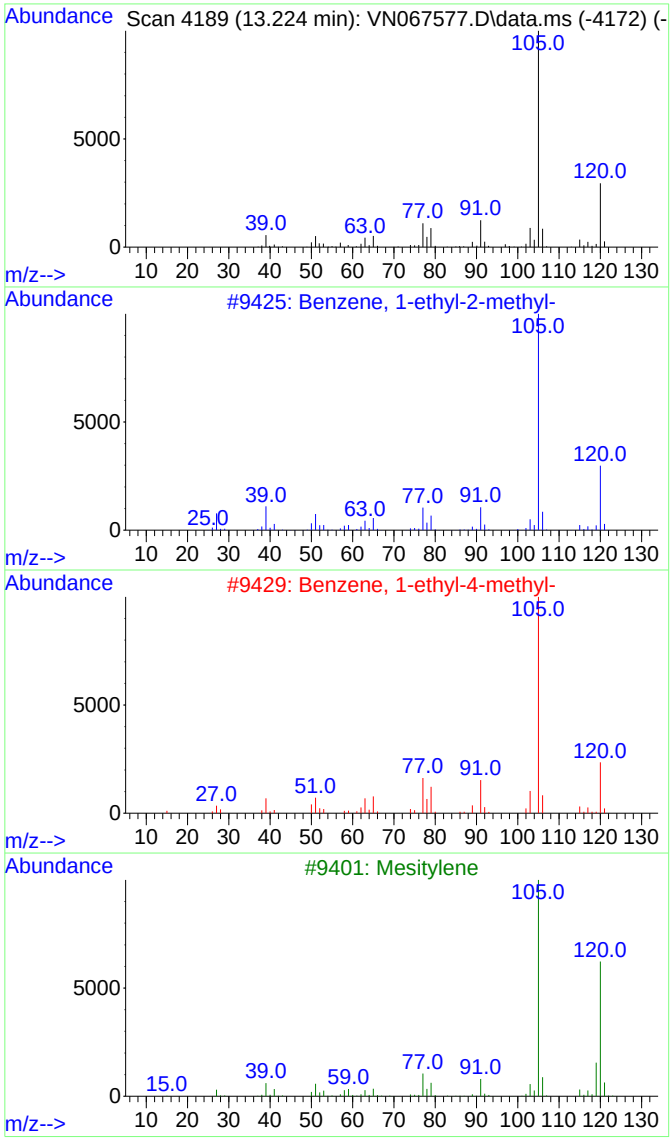
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

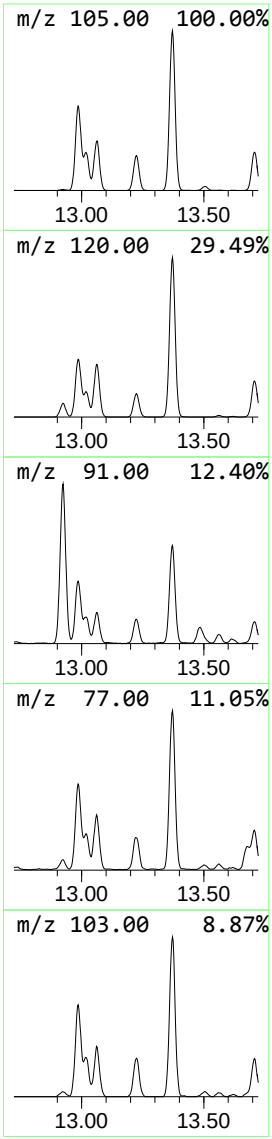
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	9.75 ug/l	587091	1,4-Dichlorobenzene-d4	13.678

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	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_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

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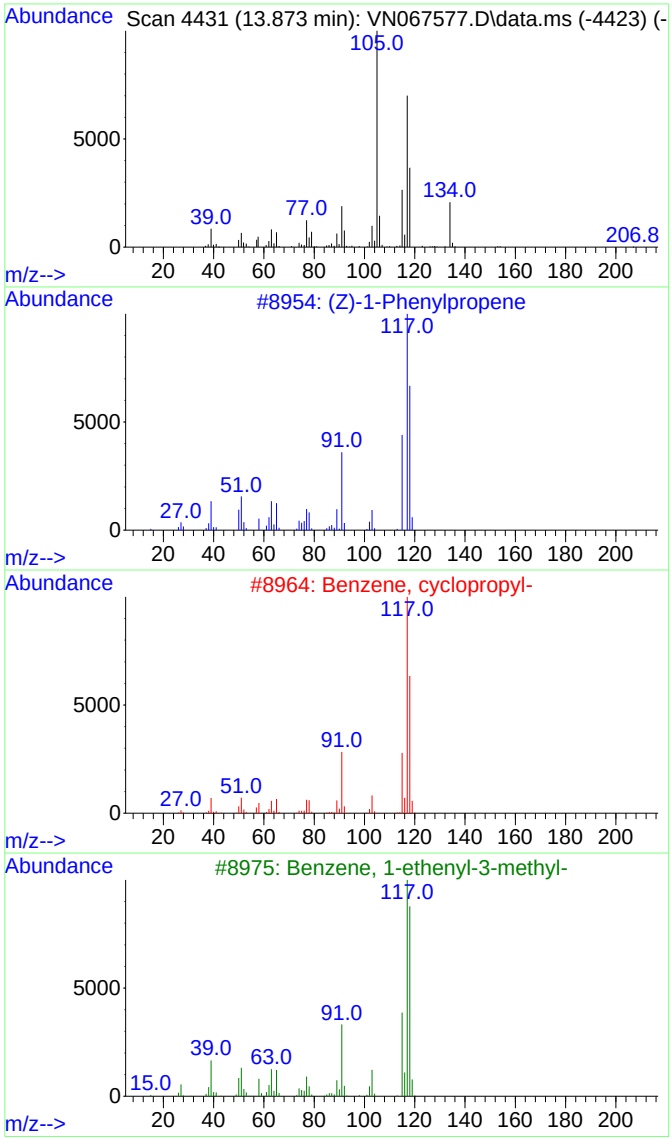
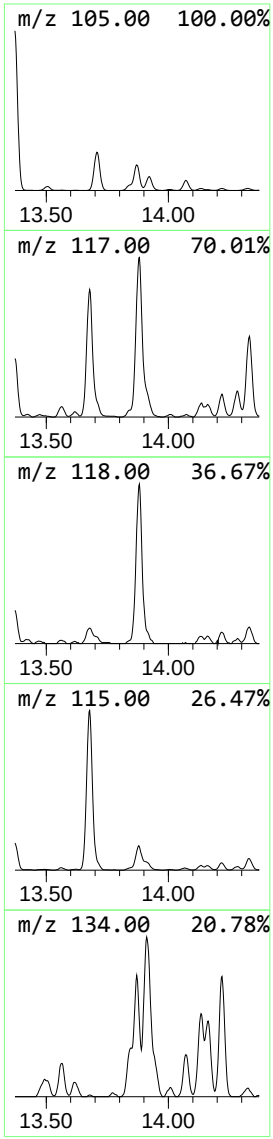
Peak Number 8 (Z)-1-Phenylpropene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	9.76 ug/l	587910	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	50
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	49
3	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	46
4	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	46
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

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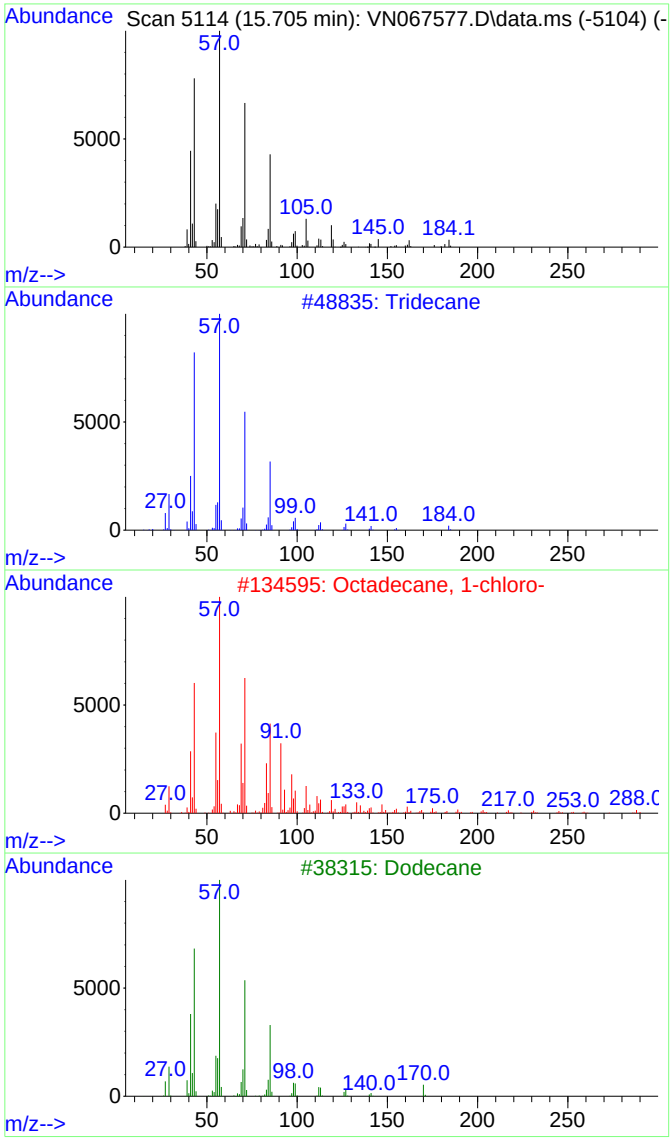
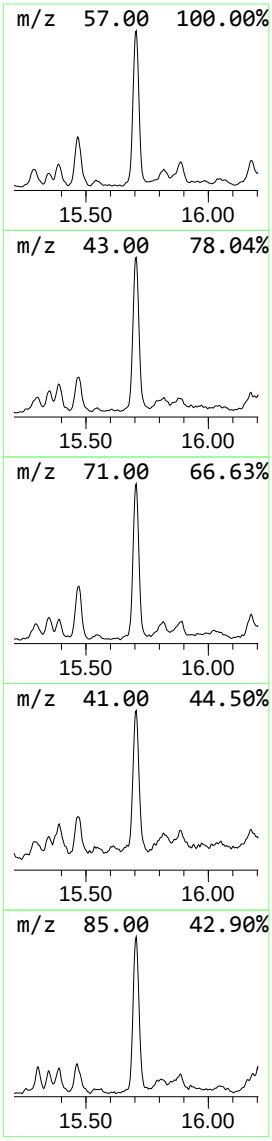
Peak Number 9 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.705	8.12 ug/l	488915	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	72
3	Dodecane	170	C12H26	000112-40-3	64
4	Tetradecane	198	C14H30	000629-59-4	59
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

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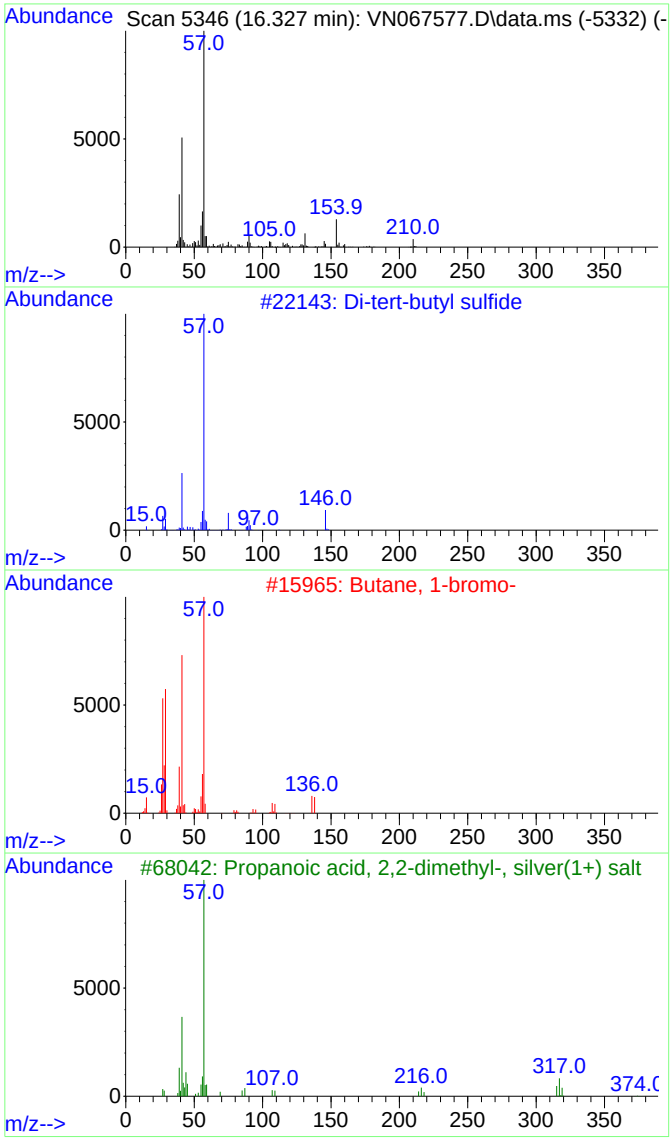
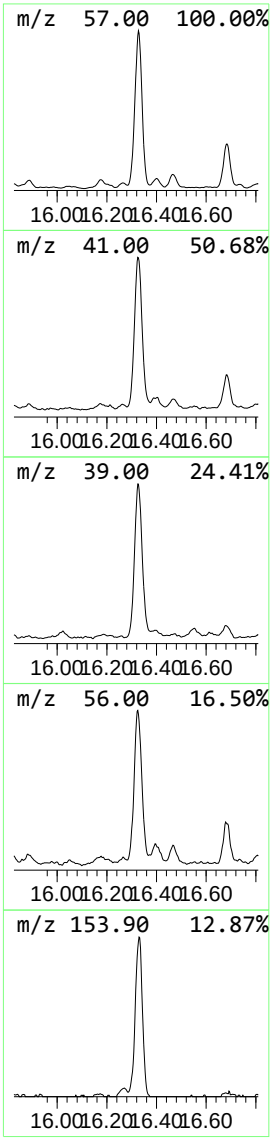
Peak Number 10 unknown16.327 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	16.08 ug/l	968413	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	47
2	Butane, 1-bromo-	136	C4H9Br	000109-65-9	35
3	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	32
4	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	27
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN063021\
Data File : VN067577.D
Acq On : 30 Jun 2021 17:19
Operator : JC/MD
Sample : M2882-01
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SPILL-COMP-31277-AUD-1077

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.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
2-Butene	2.413	6.7	ug/l	137552	1	8.080	1034080	50.0
Hexane, 3-methyl-	8.284	10.3	ug/l	213398	1	8.080	1034080	50.0
Heptane	8.820	9.1	ug/l	246689	2	8.965	1349160	50.0
Octane, 2-methyl-	11.529	11.7	ug/l	451281	3	11.749	1931570	50.0
Octane, 3-methyl-	11.628	6.1	ug/l	234093	3	11.749	1931570	50.0
Benzene, 1-ethy...	12.986	21.5	ug/l	1293850	4	13.678	3011380	50.0
Benzene, 1-ethy...	13.224	9.8	ug/l	587091	4	13.678	3011380	50.0
(Z)-1-Phenylpro...	13.873	9.8	ug/l	587910	4	13.678	3011380	50.0
Tridecane	15.705	8.1	ug/l	488915	4	13.678	3011380	50.0
unknown16.327	16.327	16.1	ug/l	968413	4	13.678	3011380	50.0