LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

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\82N061722W.M
Title : SW846 8260

Signal : TIC: VN073032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	48	58	64	rBV	263870	403422	2.93%	0.483%
2	2.405	81	88	98	rBV	1097402	1724029	12.52%	2.062%
3	3.087	194	204	239	rBV	4872869	11018826	80.05%	13.181%
4	3.457	257	267	282	rBV	1625292	3979683	28.91%	4.761%
5	3.663	292	302	315	rVB	380797	939448	6.82%	1.124%
6	3.834	315	331	339	rBV	184509	509640	3.70%	0.610%
7	3.934	339	348	363	rVB	782070	2103302	15.28%	2.516%
8	4.187	379	391	410	rVB4	75128	297506	2.16%	0.356%
9	4.881	488	509	518	rBV3	139434	521014	3.78%	0.623%
10	4.998	518	529	534	rBV3	182877	623466	4.53%	0.746%
11	5.104	534	547	558	rVV2	645908	2550735	18.53%	3.051%
12	5.540	605	621	635	rBV2	226107	797364	5.79%	0.954%
13	6.034	696	705	720	rVB3	45533	145558	1.06%	0.174%
14	6.387	754	765	777	rVV	313099	935714	6.80%	1.119%
15	6.522	777	788	796	rVV2	200700	618587	4.49%	0.740%
16	6.616	796	804	813	rVV2	208961	659151	4.79%	0.789%
17	6.710	813	820	830	rVV2	107652	335993	2.44%	0.402%
18	6.816	830	838	855	rVB3	182751	554788	4.03%	0.664%
19	7.069	868	881	890	rBV	1387679	4139978	30.08%	4.952%
20	7.769	982	1000	1010	rBV	173830	492030	3.57%	0.589%
21	7.951	1021	1031	1036	rBV	201320	501349	3.64%	0.600%
22	8.022	1036	1043	1053	rVV2	867597	2233627	16.23%	2.672%
23	8.104	1053	1057	1070	rVB5	66210	190968	1.39%	0.228%
24	8.381	1094	1104	1112	rBV3	372917	1058050	7.69%	1.266%
25	8.463	1112	1118	1122	rVV	241902	509612	3.70%	0.610%
26	8.516	1122	1127	1134	rVB	308455	690838	5.02%	0.826%
27	8.898	1181	1192	1205	rBV	596070	1341350	9.74%	1.605%
28	9.392	1262	1276	1284	rBV2	99590	316312	2.30%	0.378%
29	9.733	1326	1334	1336	rBV2	105984	189268	1.37%	0.226%
30	9.763	1336	1339	1346	rVB2	115054	216705	1.57%	0.259%
31	9.904	1355	1363	1371	rBV	293825	559467	4.06%	0.669%
32	10.139	1395	1403	1404	rBV2	131780	222244	1.61%	0.266%
33	10.169	1404	1408	1416	rVV	313962	582836	4.23%	0.697%
34	10.257	1416	1423	1430	rVB	138760	261742	1.90%	0.313%
35	10.375	1435	1443	1449	rBV	737905	1369957	9.95%	1.639%
36	10.439	1449	1454	1459	rVV	1053130	1945039	14.13%	2.327%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

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\82N061722W.M
Title : SW846 8260

37	10.486	1459	1462	1470	rVB	295012	478769	3.48%	0.573%
38	11.145	1564	1574	1585	rBV4	110623	231849	1.68%	0.277%
39	11.680	1657	1665	1674	rBV	846820	1472998	10.70%	1.762%
40	11.780	1674	1682	1691	rVV	2370961	3878897	28.18%	4.640%
41	11.886	1692	1700	1712	rBV	7174416	13765232	100.00%	16.467%
42	12.216	1748	1756	1762	rBV	105633	174822	1.27%	0.209%
43	12.516	1794	1807	1816	rBV	1078598	1789452	13.00%	2.141%
44	12.669	1825	1833	1843	rVB	666031	1121354	8.15%	1.341%
45	12.857	1857	1865	1871	rBV	1374634	2173476	15.79%	2.600%
46	12.998	1884	1889	1896	rVB	320099	515624	3.75%	0.617%
47	13.157	1907	1916	1925	rBV	777050	1272424	9.24%	1.522%
48	13.610	1986	1993	2003	rBV2	880369	1883048	13.68%	2.253%
49	13.810	2016	2027	2043	rVB	3277928	5636729	40.95%	6.743%
50	14.151	2079	2085	2090	rBV	158597	238261	1.73%	0.285%
51	14.263	2099	2104	2112	rVB	292226	491889	3.57%	0.588%
52	14.745	2178	2186	2192	rBV	157229	254152	1.85%	0.304%
53	14.863	2194	2206	2213	rBV2	319456	594844	4.32%	0.712%
54	15.427	2293	2302	2316	rBV	1074498	2081469	15.12%	2.490%

Sum of corrected areas: 83594887

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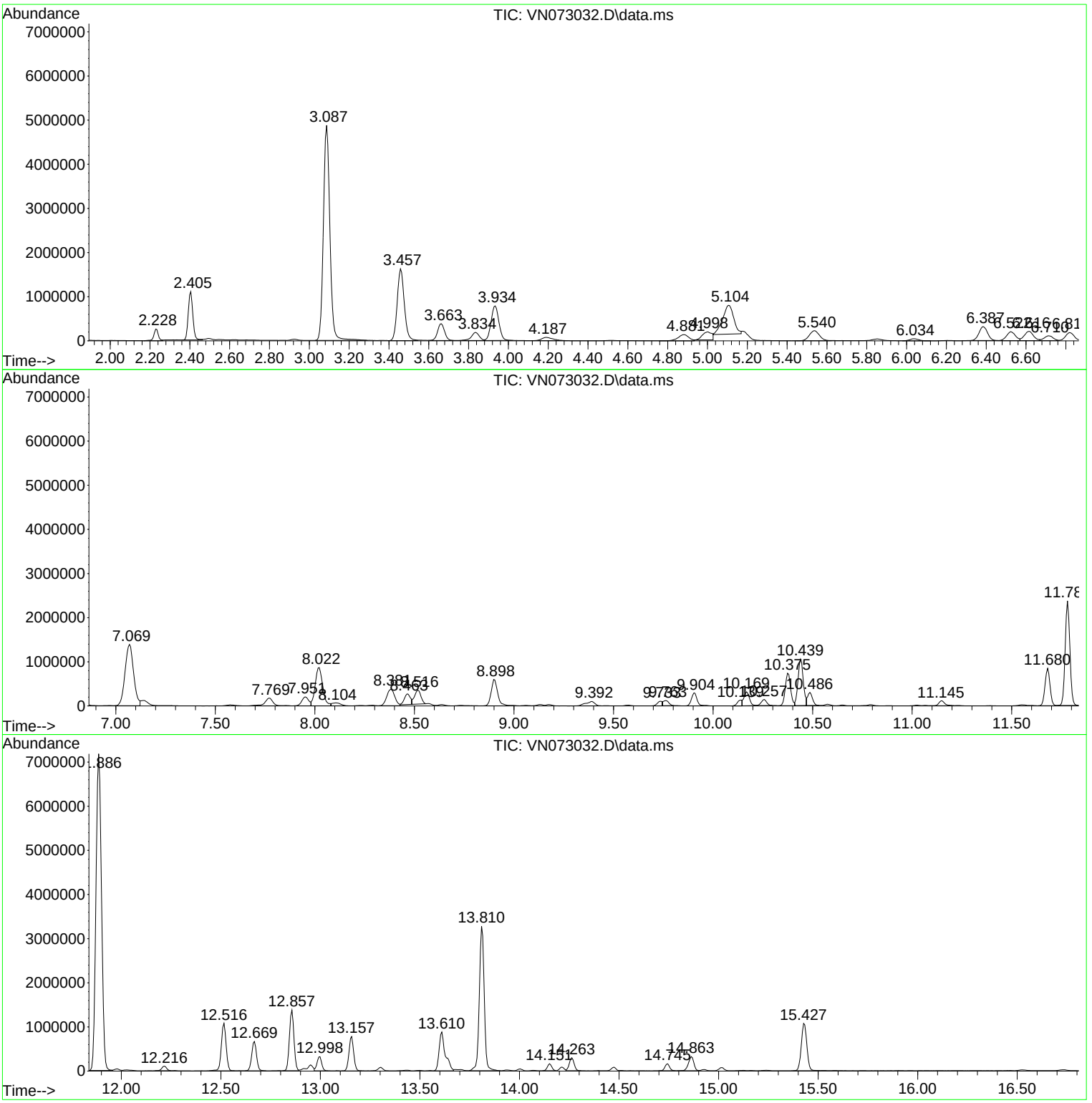
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

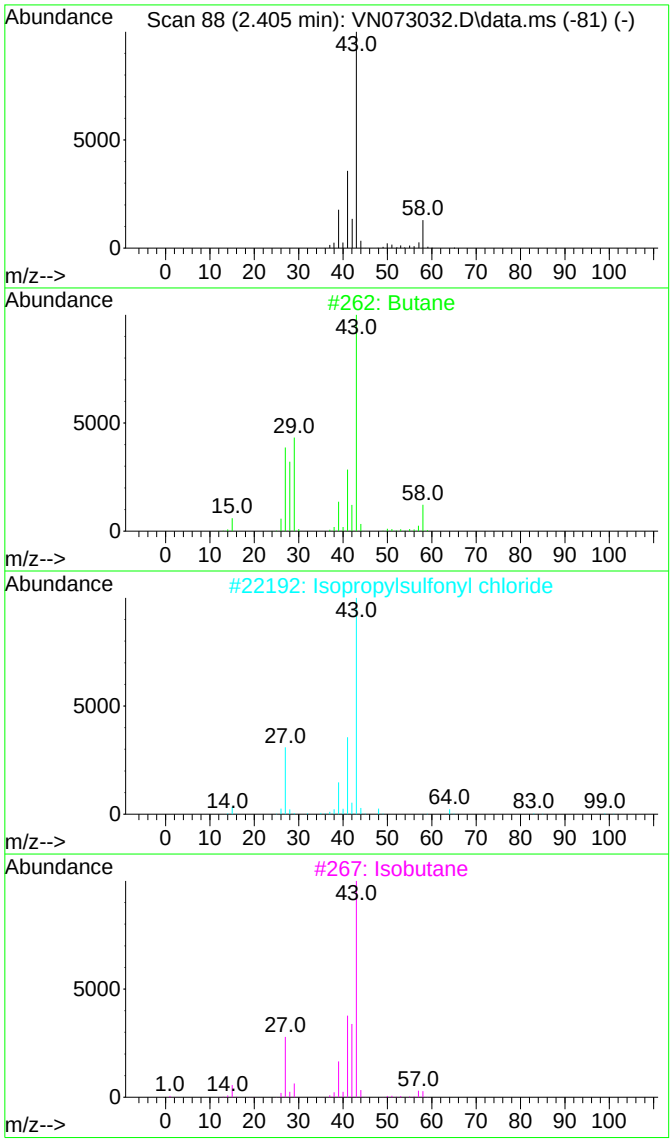
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

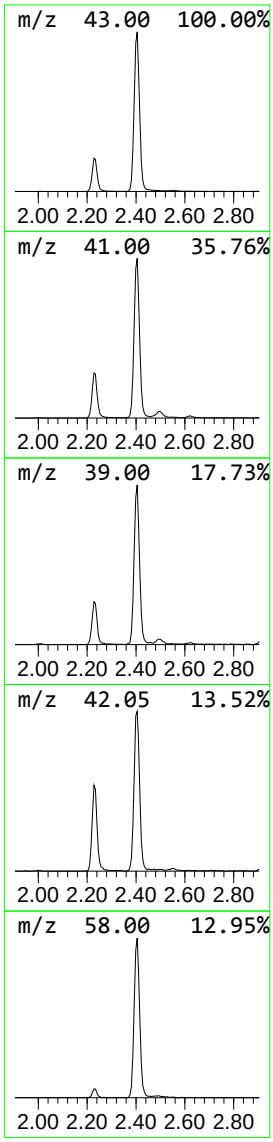
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.405	38.59 ug/l	1724030	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

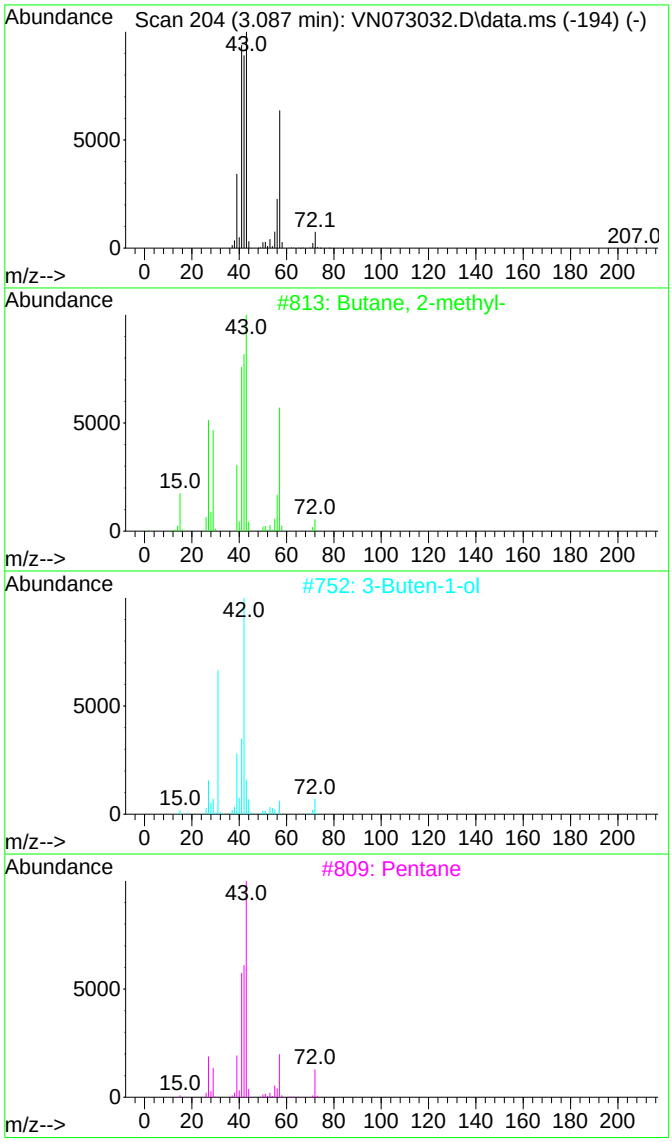
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

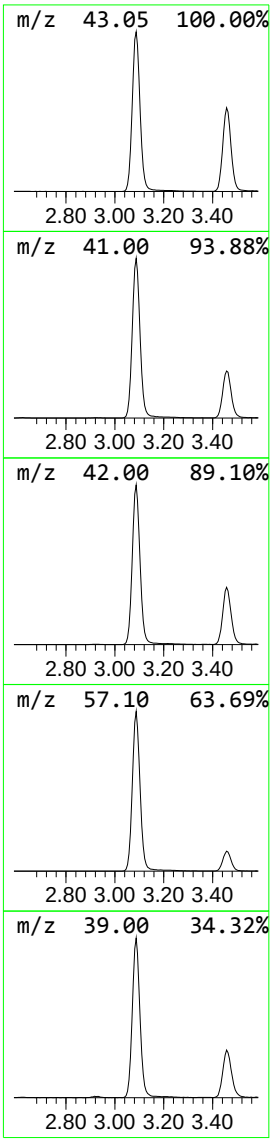
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	246.66 ug/l	11018800	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	1-Butene	56	C4H8	000106-98-9	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

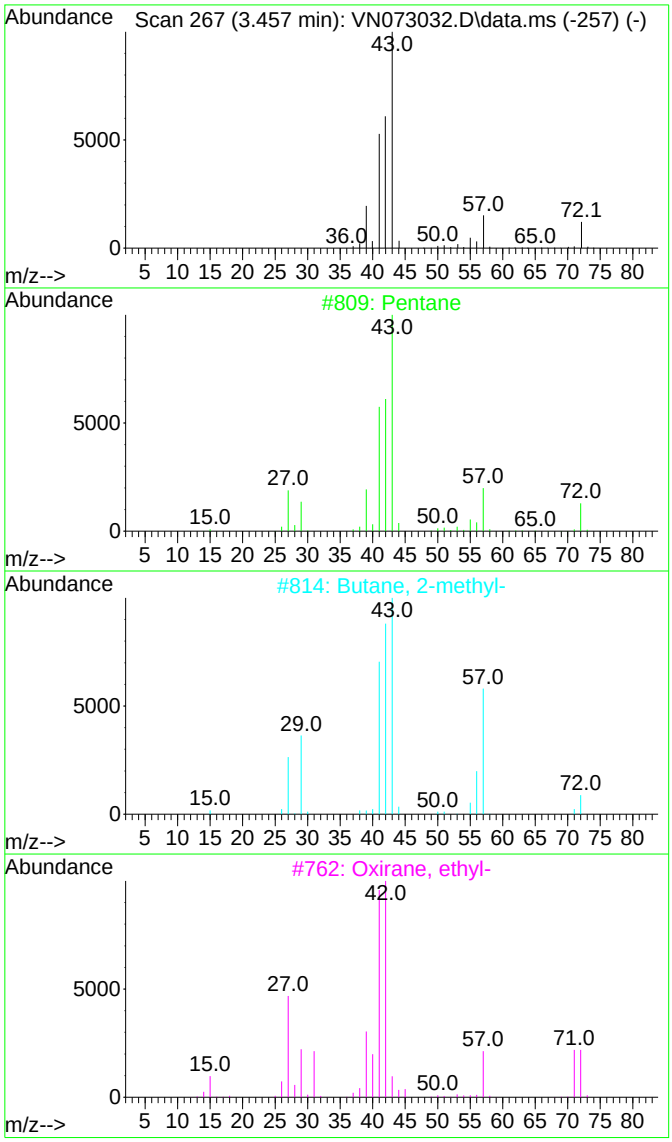
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

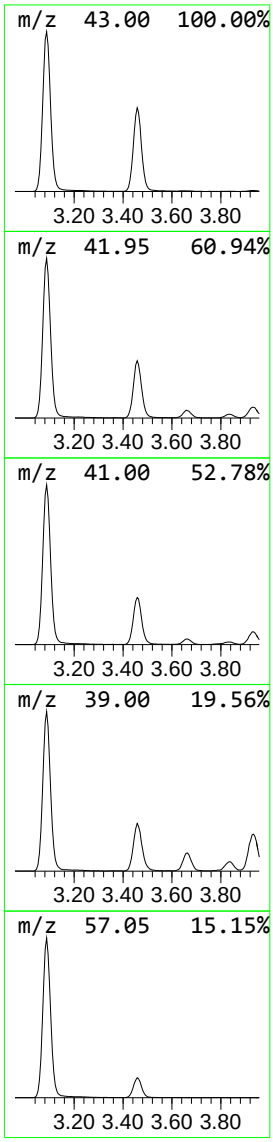
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	89.09 ug/l	3979680	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

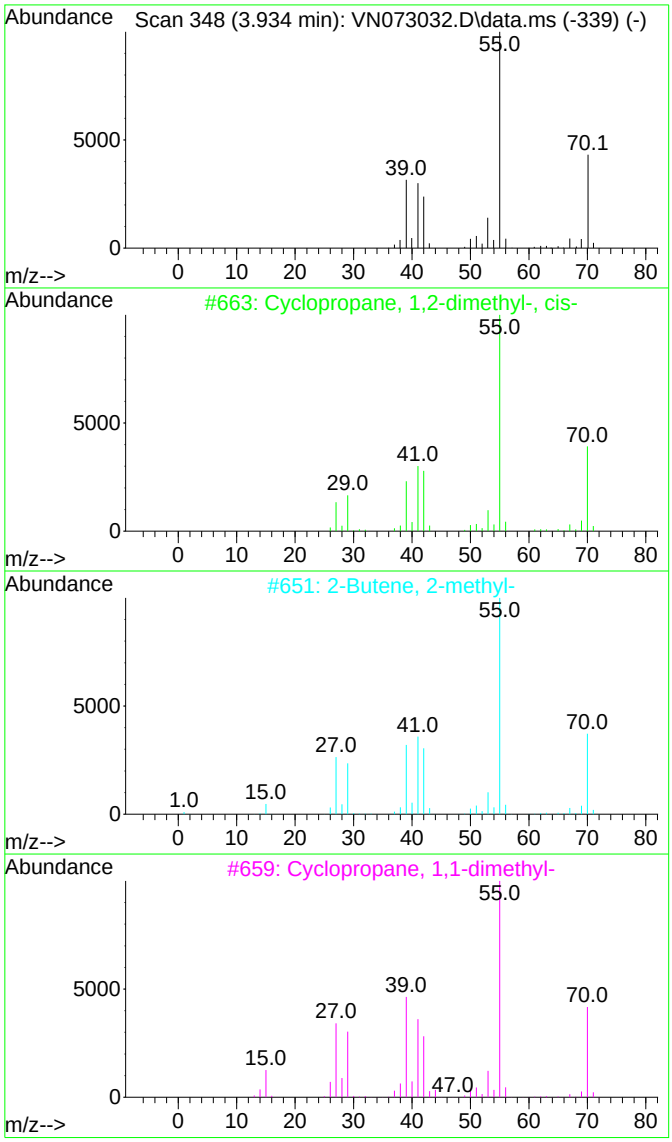
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

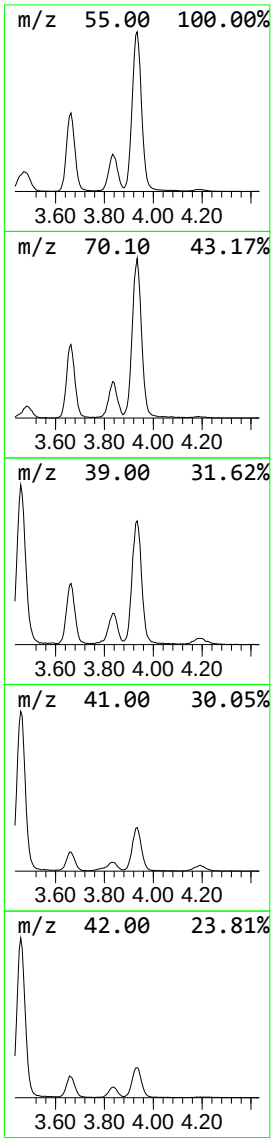
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.934	47.08 ug/l	2103300	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
5	2-Methyl-1-butene	70	C5H10	000563-46-2	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

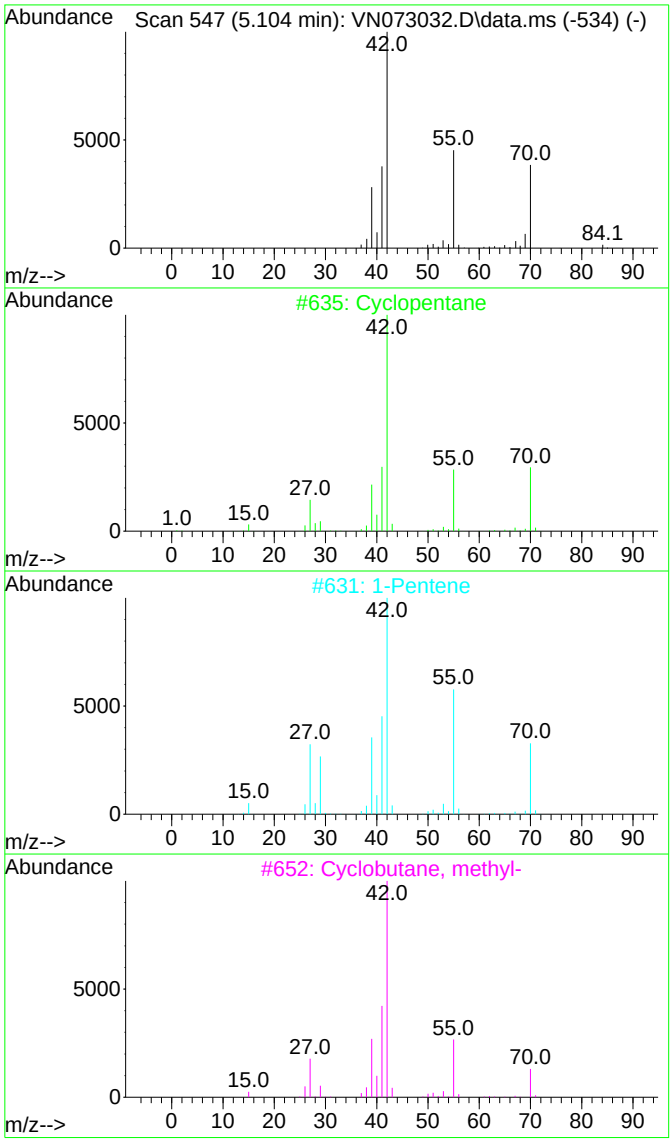
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

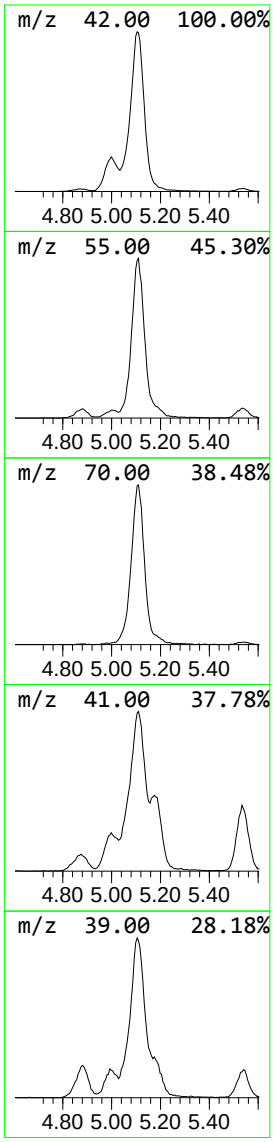
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	57.10 ug/l	2550740	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	56
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	53
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	Methyl propargyl ether	70	C4H6O	000627-41-8	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

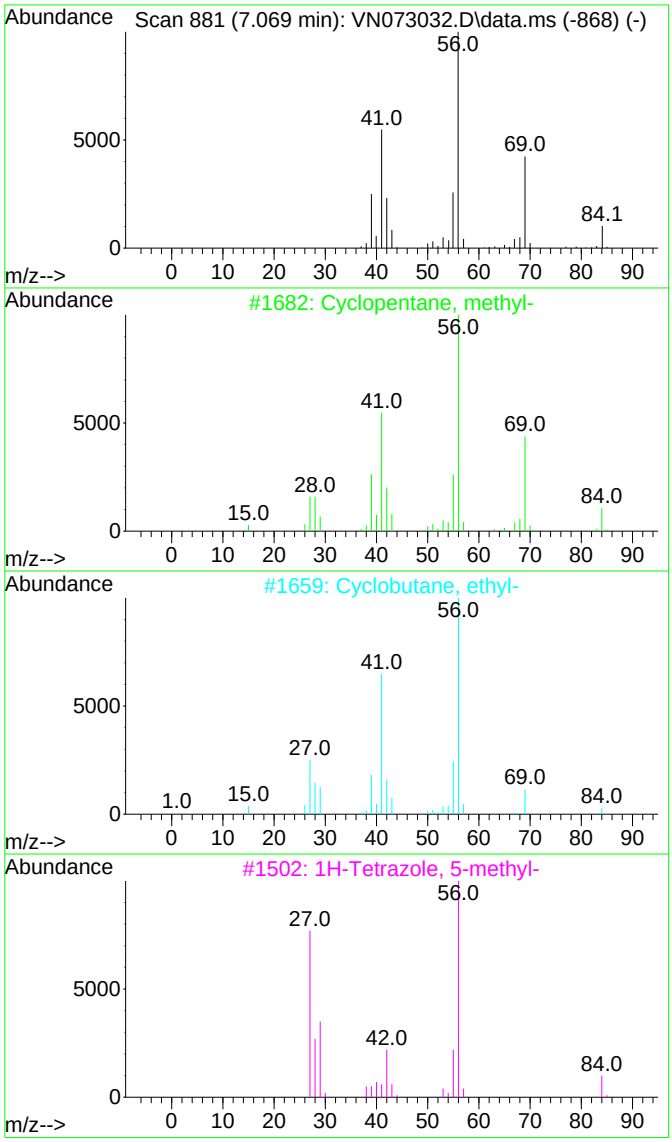
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

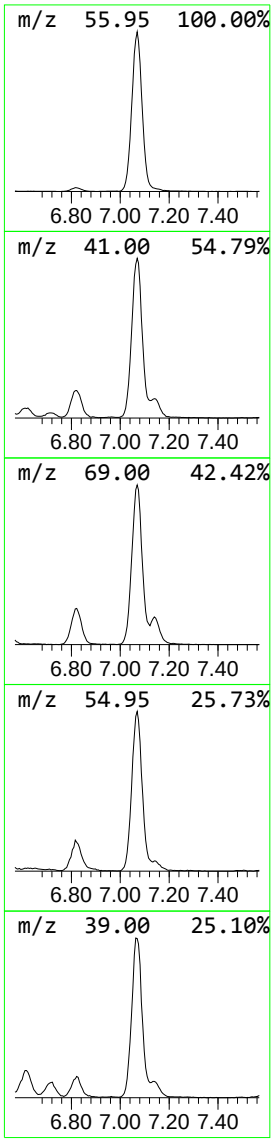
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	92.67 ug/l	4139980	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclohexane	84	C6H12	000110-82-7	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64





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Data File : VN073032.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

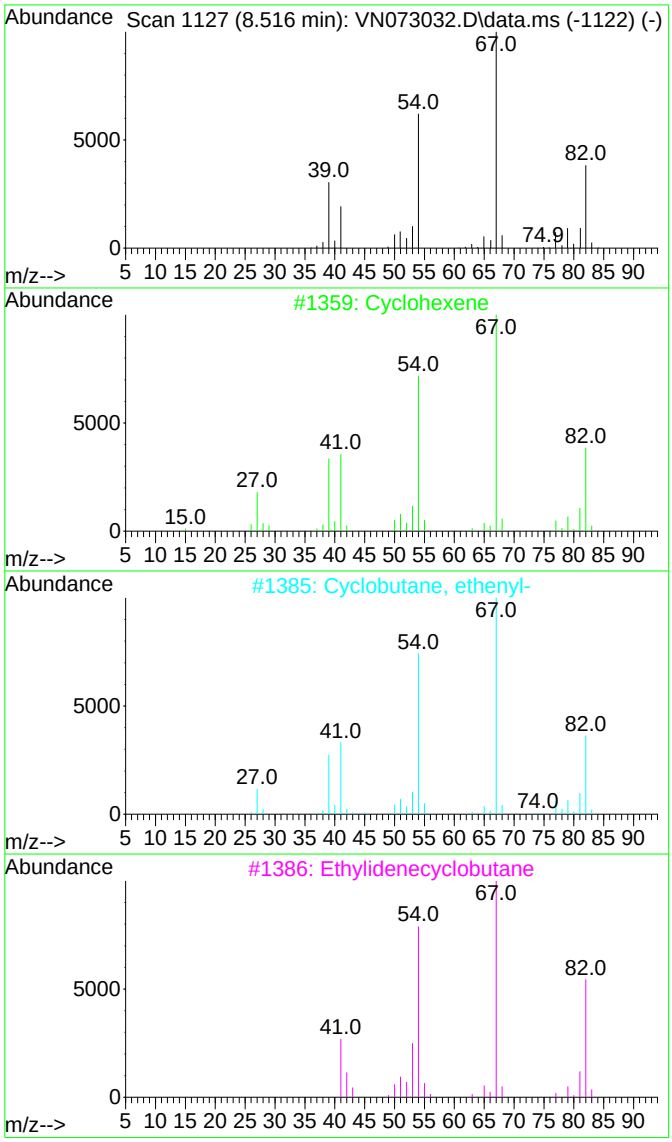
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

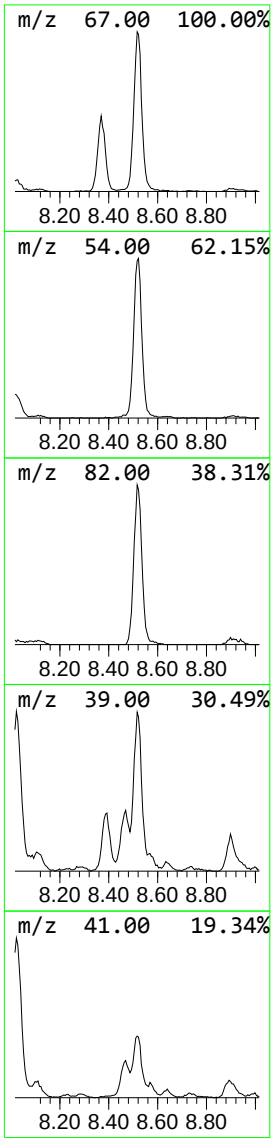
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.516	25.75 ug/l	690838	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	93
2	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	87
4	Cyclopentane, methylene-	82	C6H10	001528-30-9	68
5	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

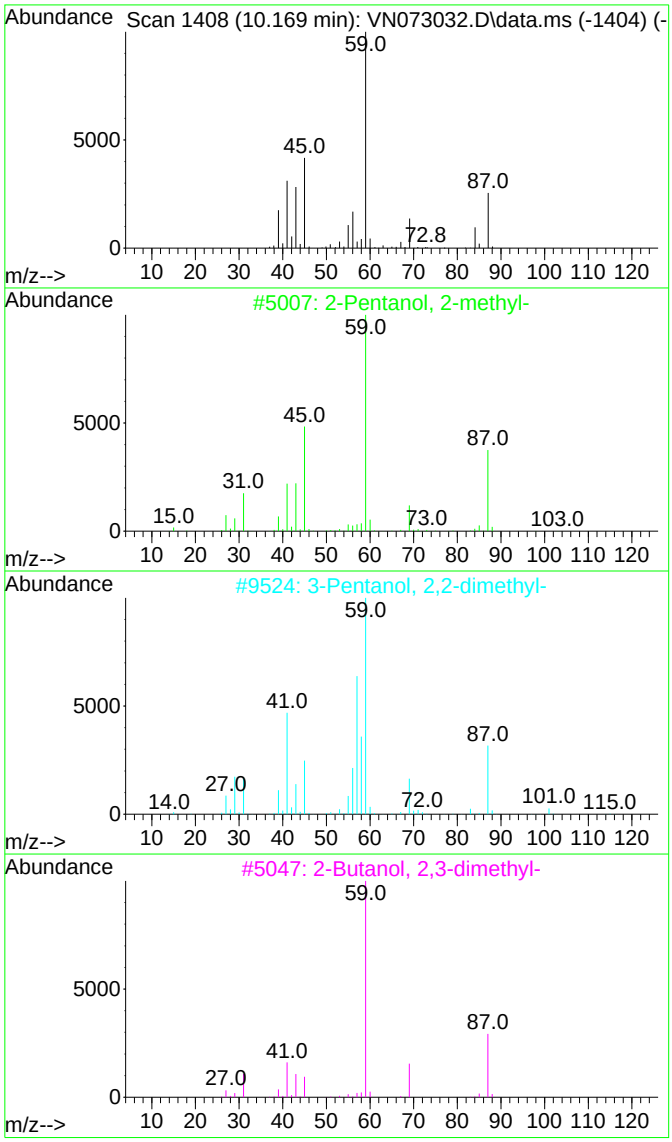
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

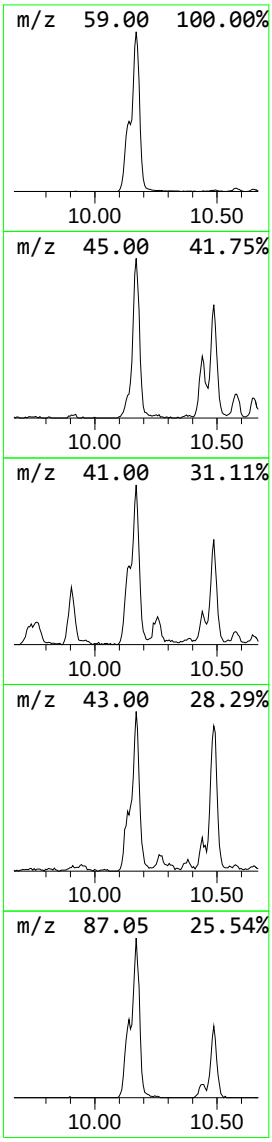
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Pentanol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	21.73 ug/l	582836	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	53
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	40
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	38
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	37





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Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

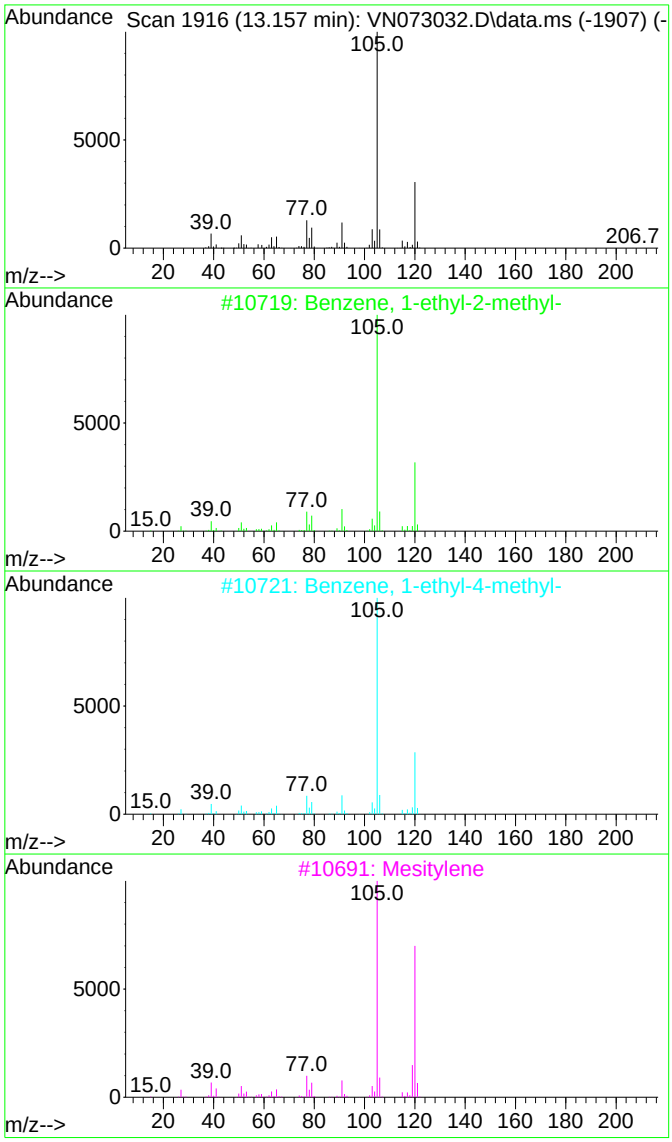
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

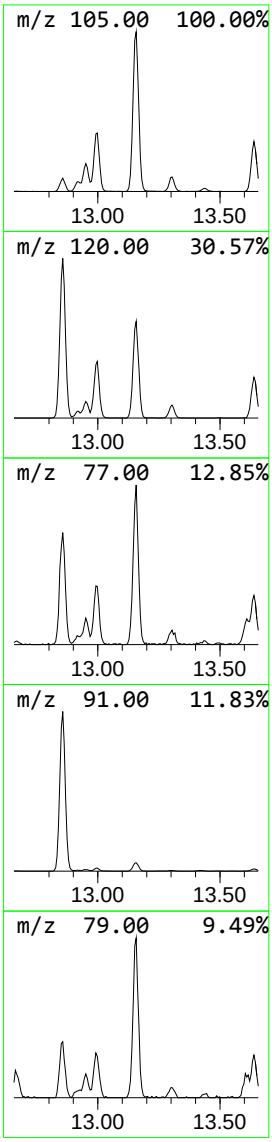
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	33.79 ug/l	1272420	1,4-Dichlorobenzene-d4	13.610

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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

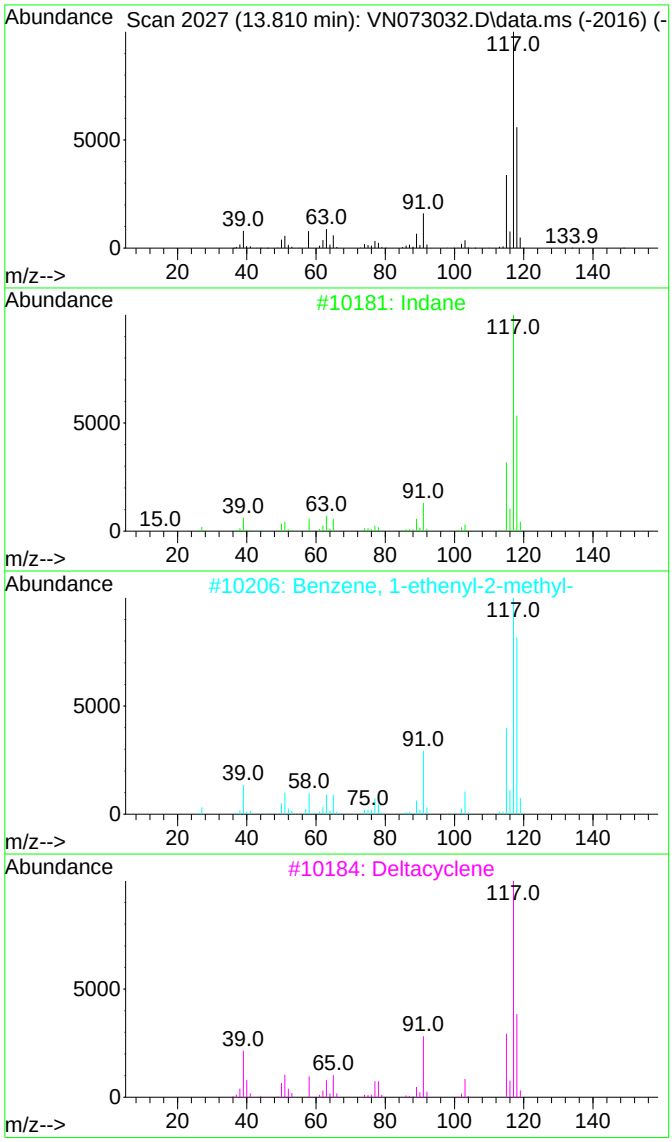
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

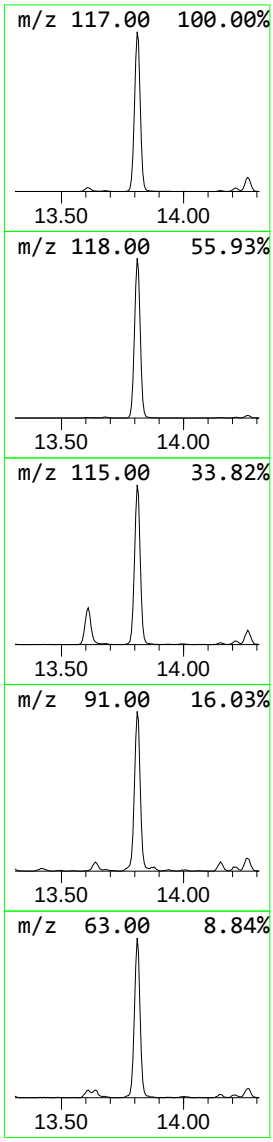
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	149.67 ug/l	5636730	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
3	Deltacyclene	118	C9H10	007785-10-6	72
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062222\
Data File : VN073032.D
Acq On : 22 Jun 2022 18:07
Operator : JC\MD
Sample : N3381-16
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PZ-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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	2.405	38.6	ug/l	1724030	1	8.016	2233630	50.0
Butane, 2-methyl-	3.087	246.7	ug/l	11018800	1	8.016	2233630	50.0
Pentane	3.457	89.1	ug/l	3979680	1	8.016	2233630	50.0
Cyclopropane, 1...	3.934	47.1	ug/l	2103300	1	8.016	2233630	50.0
Cyclopentane	5.104	57.1	ug/l	2550740	1	8.016	2233630	50.0
Cyclopentane, m...	7.069	92.7	ug/l	4139980	1	8.016	2233630	50.0
Cyclohexene	8.516	25.8	ug/l	690838	2	8.898	1341350	50.0
2-Pentanol, 2-m...	10.169	21.7	ug/l	582836	2	8.898	1341350	50.0
Benzene, 1-ethy...	13.157	33.8	ug/l	1272420	4	13.610	1883050	50.0
Indane	13.810	149.7	ug/l	5636730	4	13.610	1883050	50.0