LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030304.D
Acq On : 29 Jul 2022 15:45
Operator : JC/MD
Sample : N3861-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.234	20	24	27	rBV	10651	15155	1.14%	0.209%
2	1.746	103	108	114	rVB	47061	61782	4.63%	0.851%
3	2.337	196	205	210	rBV	30493	59875	4.49%	0.824%
4	2.538	231	238	246	rBV	12068	24014	1.80%	0.331%
5	2.776	267	277	289	rBV	122536	276761	20.75%	3.810%
6	3.105	322	331	341	rBV4	18795	53039	3.98%	0.730%
7	4.215	500	513	522	rBV2	21374	60584	4.54%	0.834%
8	4.306	522	528	537	rVB4	7069	19047	1.43%	0.262%
9	4.581	564	573	585	rBV2	10011	35350	2.65%	0.487%
10	5.129	650	663	665	rBV6	6146	15824	1.19%	0.218%
11	5.391	691	706	716	rBV3	143608	424749	31.84%	5.847%
12	5.556	724	733	743	rBV	148623	423448	31.74%	5.829%
13	5.849	771	781	791	rBV7	9536	31004	2.32%	0.427%
14	5.964	791	800	812	rBV	177101	465594	34.90%	6.410%
15	6.251	840	847	856	rVB2	16783	51381	3.85%	0.707%
16	6.361	856	865	875	rVB4	14988	44469	3.33%	0.612%
17	6.769	922	932	944	rBV	256741	611190	45.82%	8.414%
18	7.367	1020	1030	1041	rBV5	25034	64876	4.86%	0.893%
19	7.781	1091	1098	1105	rVB2	17387	36425	2.73%	0.501%
20	7.988	1122	1132	1141	rVB2	15349	36984	2.77%	0.509%
21	8.110	1141	1152	1162	rBV	39553	81776	6.13%	1.126%
22	8.324	1181	1187	1196	rBV5	10410	22814	1.71%	0.314%
23	8.519	1211	1219	1226	rVB4	8445	19200	1.44%	0.264%
24	8.653	1226	1241	1253	rBV	843695	1333913	100.00%	18.364%
25	8.781	1256	1262	1266	rVB3	10643	18309	1.37%	0.252%
26	8.976	1287	1294	1300	rVB6	37280	82569	6.19%	1.137%
27	9.049	1300	1306	1310	rVV3	19138	32194	2.41%	0.443%
28	9.104	1310	1315	1320	rVB2	17018	28540	2.14%	0.393%
29	9.165	1320	1325	1336	rBV	9723	18168	1.36%	0.250%
30	9.506	1377	1381	1389	rVB3	12800	23806	1.78%	0.328%
31	10.055	1462	1471	1478	rBV	584619	801968	60.12%	11.040%
32	10.964	1616	1620	1625	rBV	25037	34765	2.61%	0.479%
33	11.085	1634	1640	1646	rBV	631119	805183	60.36%	11.085%
34	11.866	1763	1768	1771	rBV	21297	28948	2.17%	0.399%
35	12.024	1789	1794	1801	rBV	784736	937254	70.26%	12.903%
36	12.244	1825	1830	1839	rVB3	14448	22463	1.68%	0.309%

LSC Area Percent Report

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Sample : N3861-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X072522W.M
Title : SW846 8260

37	12.408	1852	1857	1862	rBV2	17912	23016	1.73%	0.317%
38	12.701	1900	1905	1912	rBV4	7660	14238	1.07%	0.196%
39	12.847	1920	1929	1934	rBV	9387	15014	1.13%	0.207%
40	12.927	1934	1942	1946	rBV	53332	76594	5.74%	1.054%
41	13.579	2046	2049	2053	rBV2	12101	14552	1.09%	0.200%
42	14.323	2166	2171	2175	rBV	12751	17075	1.28%	0.235%

Sum of corrected areas: 7263910

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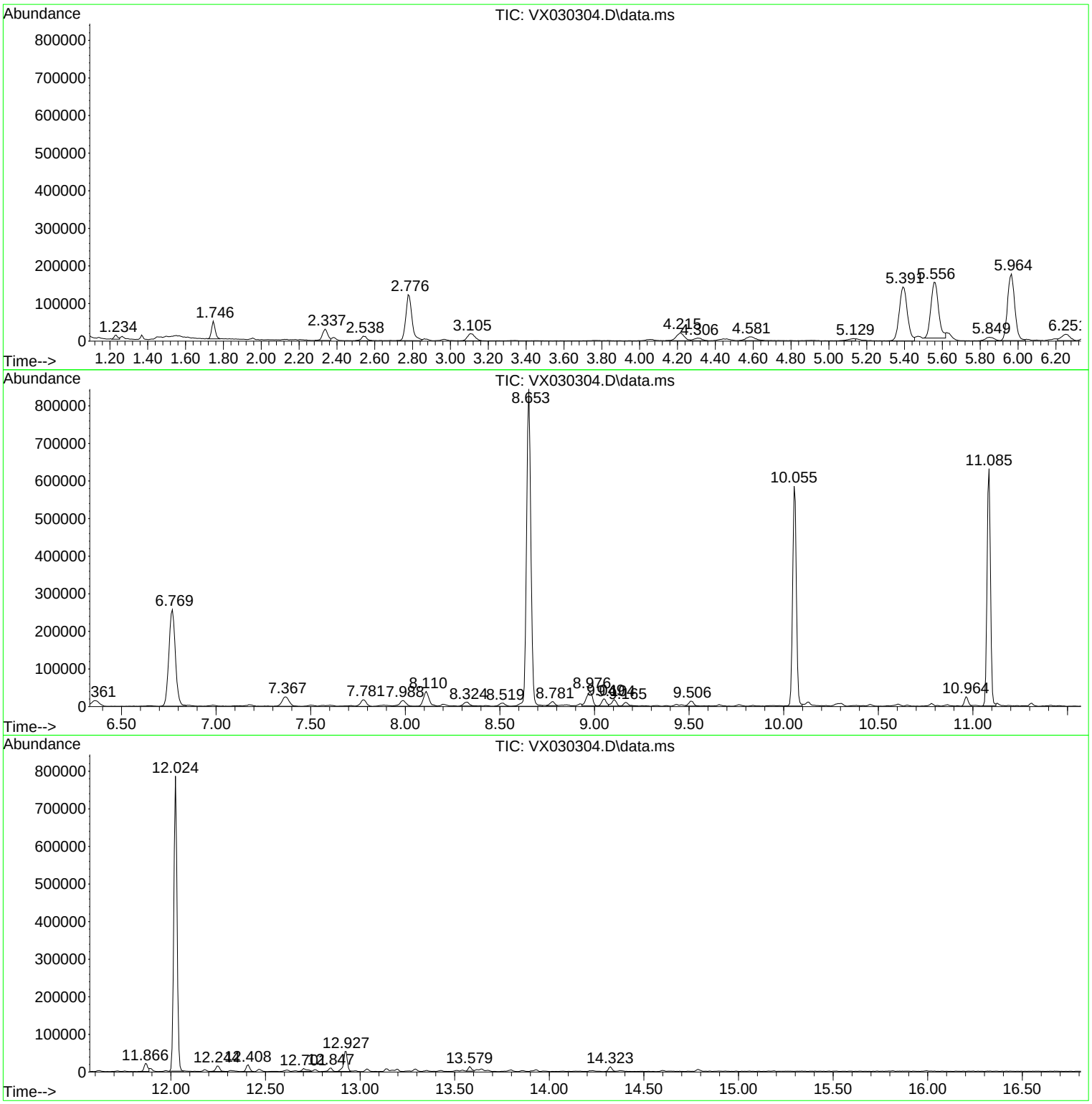
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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Data File : VX030304.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

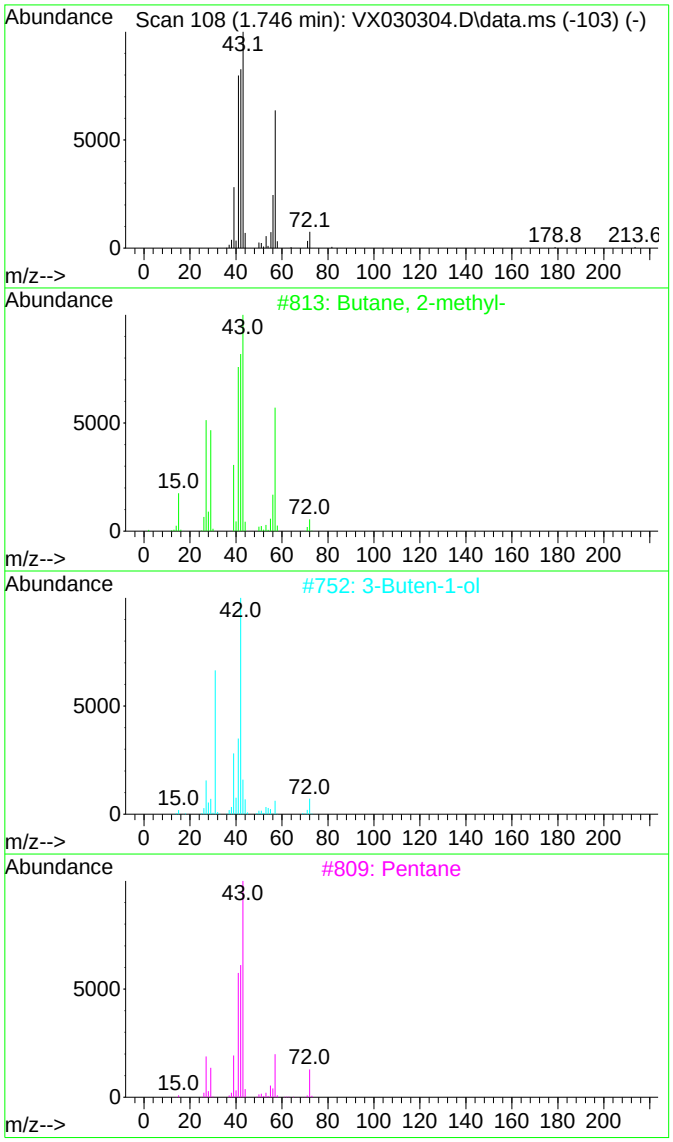
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

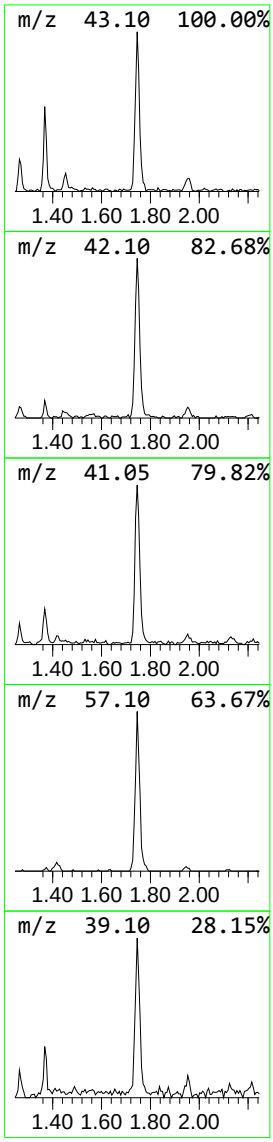
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	7.30 ug/l	61782	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	50
3	Pentane	72	C5H12	000109-66-0	45
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	39
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	38





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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

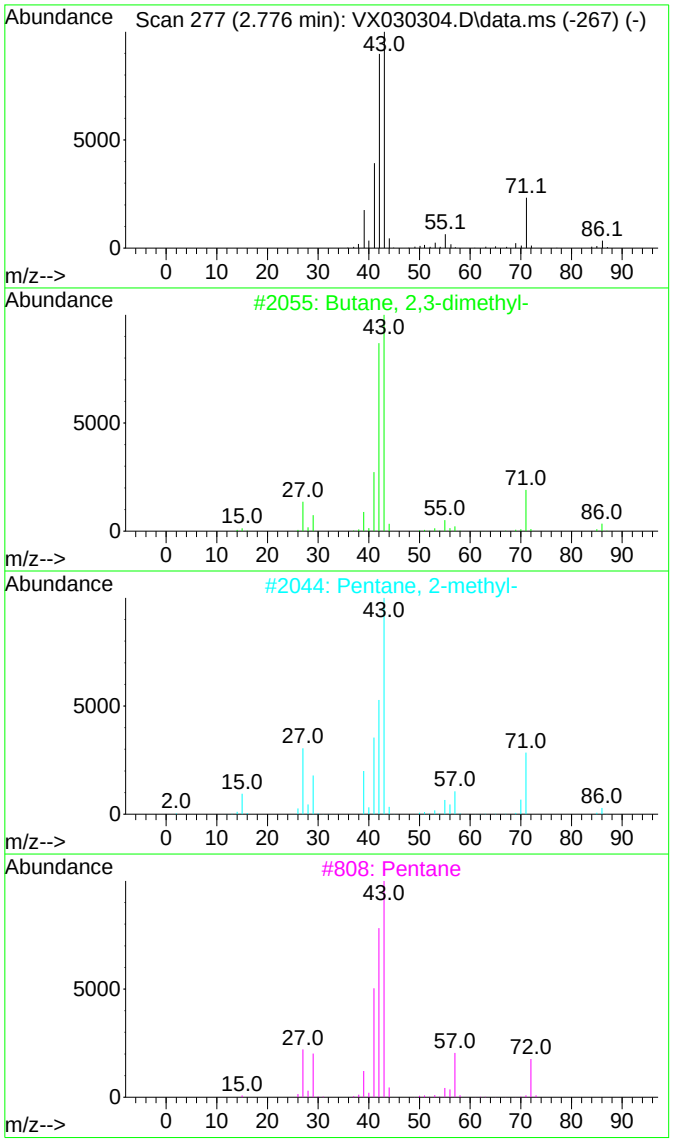
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

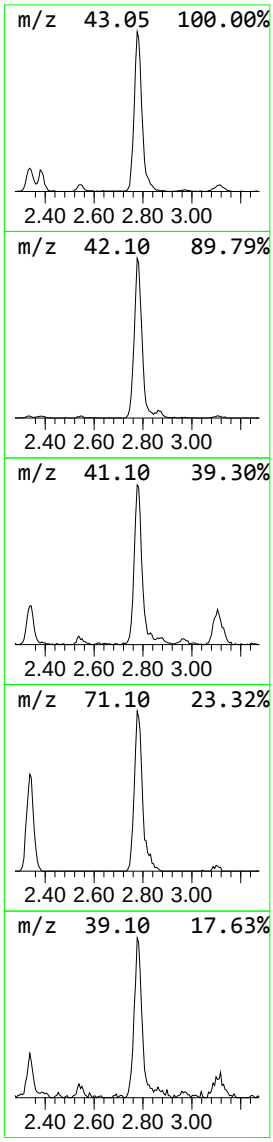
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.776	32.68 ug/l	276761	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pentane	72	C5H12	000109-66-0	45
4	Tetrahydrofuran	72	C4H8O	000109-99-9	38
5	1-Pentene	70	C5H10	000109-67-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030304.D
Acq On : 29 Jul 2022 15:45
Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

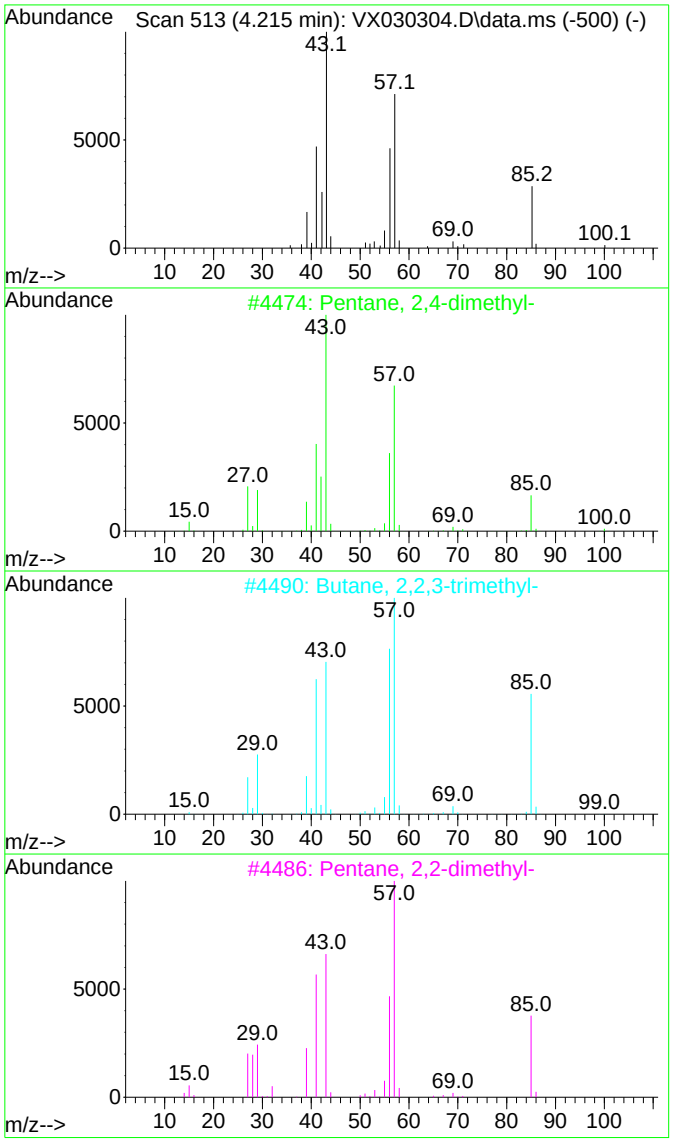
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

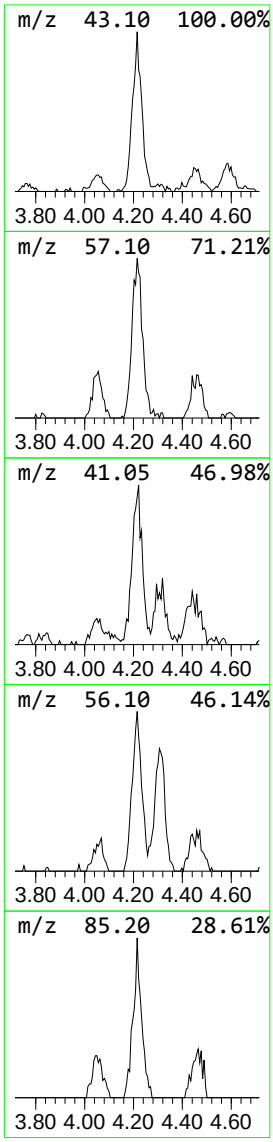
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.215	7.15 ug/l	60584	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
4	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	50
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50





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Operator : JC/MD
Sample : N3861-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

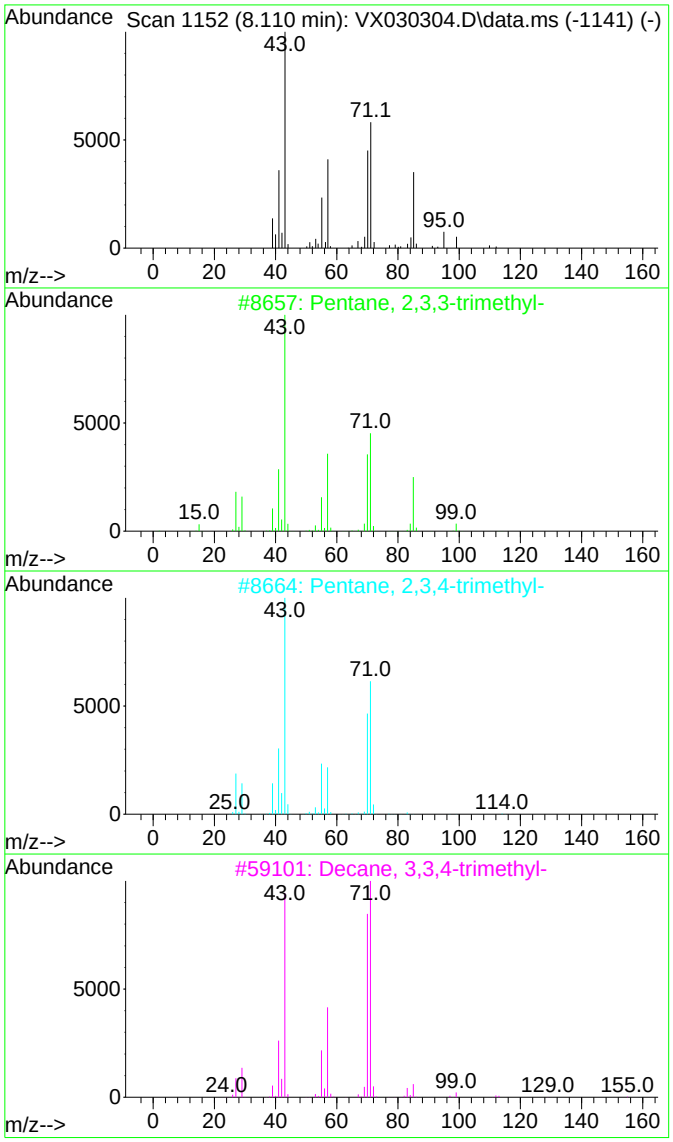
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

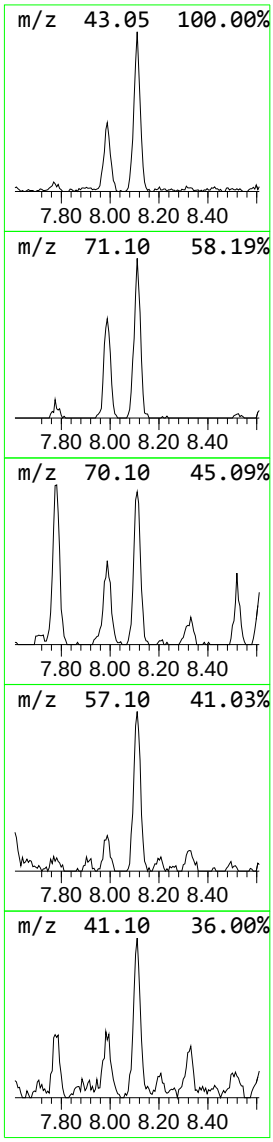
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	6.69 ug/l	81776	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	45





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Operator : JC/MD
Sample : N3861-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

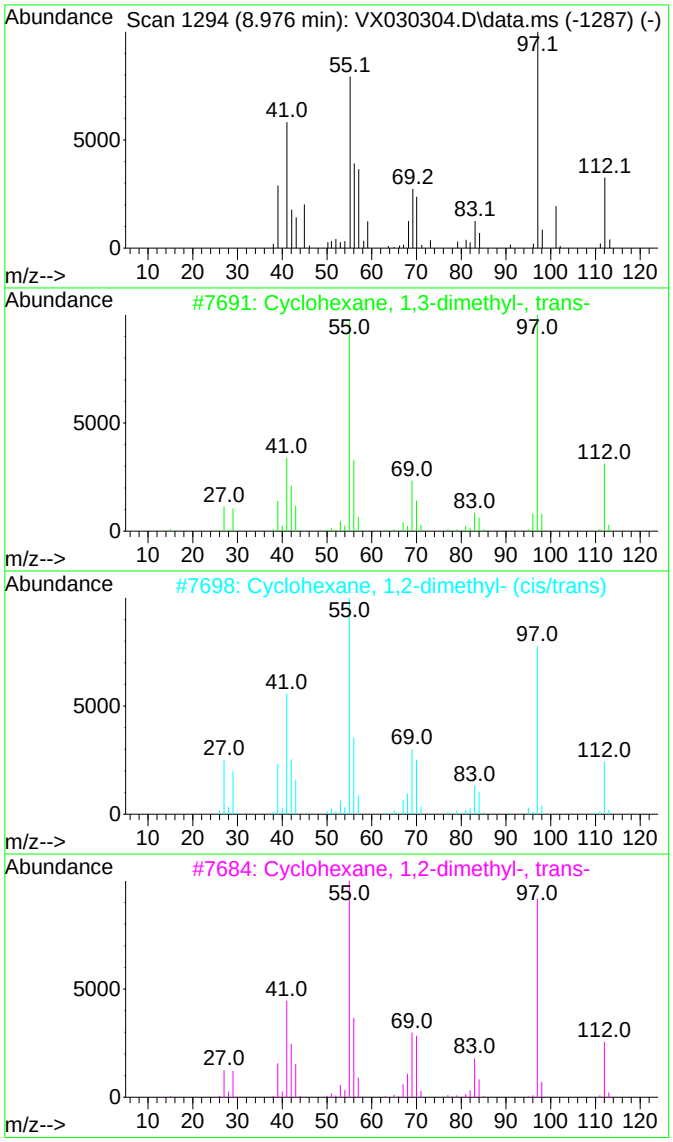
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

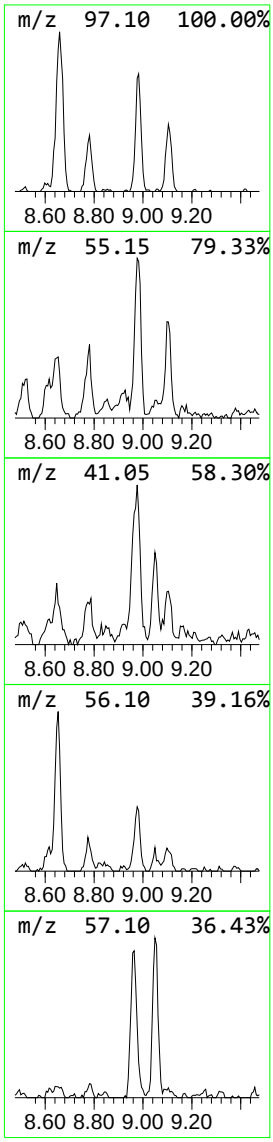
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.976	5.15 ug/l	82569	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	76
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	74
3	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	74
4	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	58
5	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	52





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methyl-	1.746	7.3	ug/l	61782	1	5.562	423448	50.0
Butane, 2,3-dim...	2.776	32.7	ug/l	276761	1	5.562	423448	50.0
Pentane, 2,4-di...	4.215	7.2	ug/l	60584	1	5.562	423448	50.0
Pentane, 2,3,3-...	8.110	6.7	ug/l	81776	2	6.769	611190	50.0
Cyclohexane, 1,...	8.976	5.2	ug/l	82569	3	10.055	801968	50.0