LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
Data File : VN064914.D
Acq On : 4 Dec 2020 13:16
Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

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\82N112320W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.978	66	74	85	rVB	7360	10423	1.09%	0.122%
2	2.435	195	216	217	rBV8	5394	10920	1.15%	0.128%
3	3.788	621	637	664	rBV2	19744	59960	6.29%	0.704%
4	7.547	1786	1806	1817	rBV2	113551	293991	30.85%	3.451%
5	7.621	1817	1829	1845	rVV	205376	498051	52.27%	5.846%
6	7.698	1845	1853	1865	rVB5	5678	12337	1.29%	0.145%
7	7.830	1879	1894	1909	rBV3	22754	52996	5.56%	0.622%
8	7.984	1926	1942	1967	rBV	117148	271273	28.47%	3.184%
9	8.396	2053	2070	2087	rBV3	27735	58884	6.18%	0.691%
10	8.547	2099	2117	2136	rBV	318203	653737	68.61%	7.674%
11	9.045	2250	2272	2282	rBV6	12547	34956	3.67%	0.410%
12	9.836	2504	2518	2526	rBV5	4750	10936	1.15%	0.128%
13	9.958	2545	2556	2570	rBV2	9917	18426	1.93%	0.216%
14	10.058	2570	2587	2597	rBV	498912	908041	95.29%	10.659%
15	10.122	2597	2607	2632	rVB	524968	952894	100.00%	11.185%
16	10.251	2639	2647	2659	rVB3	6622	11497	1.21%	0.135%
17	10.830	2812	2827	2841	rBV3	15741	31047	3.26%	0.364%
18	11.380	2985	2998	3016	rBV	469004	831531	87.26%	9.761%
19	11.482	3023	3030	3041	rVB3	7636	12689	1.33%	0.149%
20	11.595	3051	3065	3075	rBV	33237	74149	7.78%	0.870%
21	11.920	3151	3166	3181	rVB2	26034	46885	4.92%	0.550%
22	12.007	3183	3193	3208	rBV3	13717	26126	2.74%	0.307%
23	12.106	3212	3224	3241	rBV10	7541	16749	1.76%	0.197%
24	12.376	3292	3308	3330	rVB	390592	660489	69.31%	7.753%
25	12.566	3354	3367	3376	rBV	23112	35326	3.71%	0.415%
26	12.630	3376	3387	3393	rBV	86034	142789	14.98%	1.676%
27	12.662	3393	3397	3403	rVV	44270	60145	6.31%	0.706%
28	12.704	3403	3410	3421	rVB5	62311	99393	10.43%	1.167%
29	12.804	3432	3441	3450	rBV2	14662	24643	2.59%	0.289%
30	12.865	3451	3460	3469	rVV	39745	64487	6.77%	0.757%
31	13.013	3494	3506	3518	rBV	168238	274268	28.78%	3.219%
32	13.080	3520	3527	3534	rVB2	9615	14094	1.48%	0.165%
33	13.209	3563	3567	3577	rVB2	10080	11882	1.25%	0.139%
34	13.264	3577	3584	3589	rBV5	9151	12587	1.32%	0.148%

LSC Area Percent Report

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Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

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\82N112320W.M
Title : SW846 8260

35	13.318	3589	3601	3622	rBV2	514958	938857	98.53%	11.021%
36	13.428	3625	3635	3646	rVV2	41090	68663	7.21%	0.806%
37	13.489	3646	3654	3655	rVV3	13452	15685	1.65%	0.184%
38	13.515	3655	3662	3669	rVV2	61559	99265	10.42%	1.165%
39	13.560	3670	3676	3693	rVB4	44523	94417	9.91%	1.108%
40	13.646	3693	3703	3711	rBV6	10835	17750	1.86%	0.208%
41	13.714	3713	3724	3734	rBV	12736	19977	2.10%	0.234%
42	13.775	3734	3743	3748	rVV3	21846	32873	3.45%	0.386%
43	13.804	3749	3752	3761	rVB2	21342	26252	2.75%	0.308%
44	13.862	3761	3770	3781	rVB	38082	57110	5.99%	0.670%
45	13.968	3795	3803	3813	rBV2	23262	35438	3.72%	0.416%
46	14.100	3833	3844	3855	rBV4	32493	58454	6.13%	0.686%
47	14.183	3862	3870	3876	rBV2	13784	21619	2.27%	0.254%
48	14.222	3876	3882	3889	rVB2	23198	32480	3.41%	0.381%
49	14.286	3889	3902	3920	rVB3	31327	75795	7.95%	0.890%
50	14.408	3930	3940	3944	rBV10	7716	11303	1.19%	0.133%
51	14.450	3946	3953	3962	rVV3	17351	29755	3.12%	0.349%
52	14.495	3964	3967	3976	rVB6	11427	14593	1.53%	0.171%
53	14.563	3976	3988	3999	rBV4	32478	70453	7.39%	0.827%
54	14.624	4000	4007	4013	rVV4	7387	11362	1.19%	0.133%
55	14.662	4013	4019	4028	rVV5	9653	14796	1.55%	0.174%
56	14.826	4063	4070	4075	rBV7	7245	11704	1.23%	0.137%
57	14.939	4093	4105	4115	rBV8	9977	19080	2.00%	0.224%
58	15.103	4140	4156	4168	rBV	29922	58969	6.19%	0.692%
59	15.209	4181	4189	4197	rBV	5147	9620	1.01%	0.113%
60	15.855	4379	4390	4404	rVB	65590	130936	13.74%	1.537%
61	16.122	4462	4473	4486	rVV	67485	132644	13.92%	1.557%
62	16.312	4515	4532	4552	rBV2	44021	110679	11.62%	1.299%

Sum of corrected areas: 8519130

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
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Acq On : 4 Dec 2020 13:16
Operator : JC/MD
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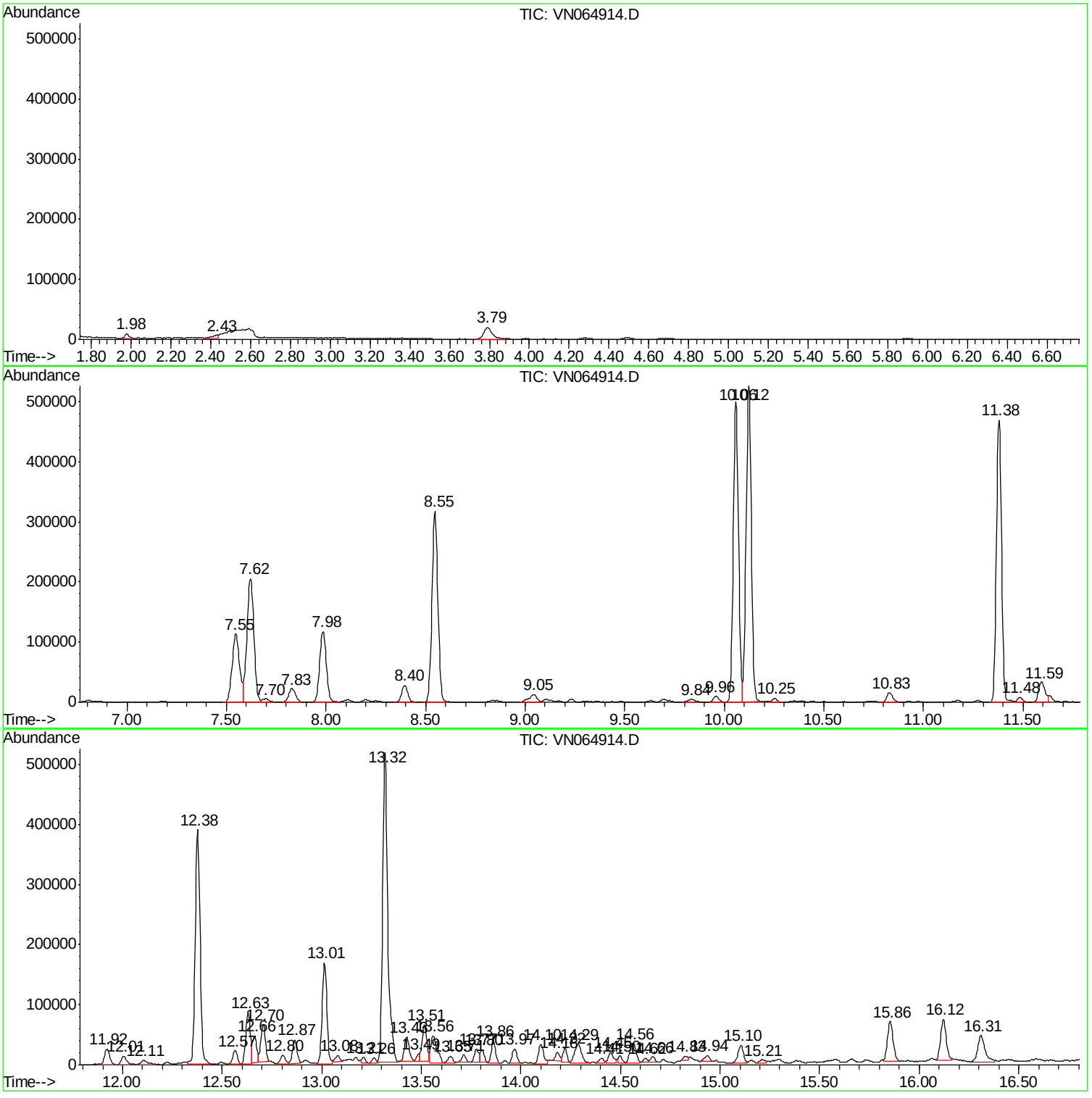
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Data File : VN064914.D
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Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

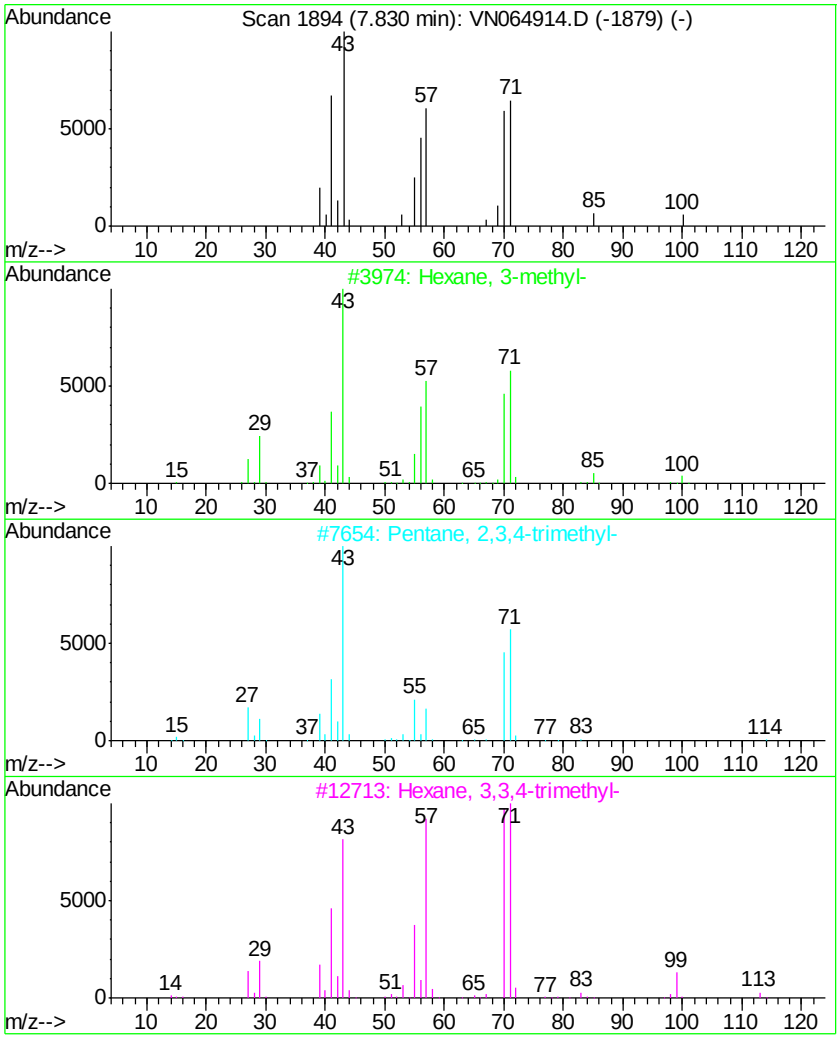
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

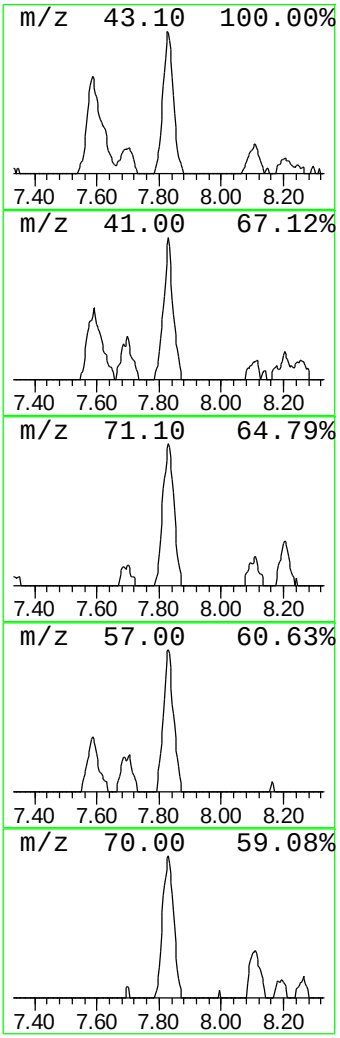
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.83	5.32 ug/l	52996	Pentafluorobenzene	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	87
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47
4	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	45
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
Data File : VN064914.D
Acq On : 4 Dec 2020 13:16
Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

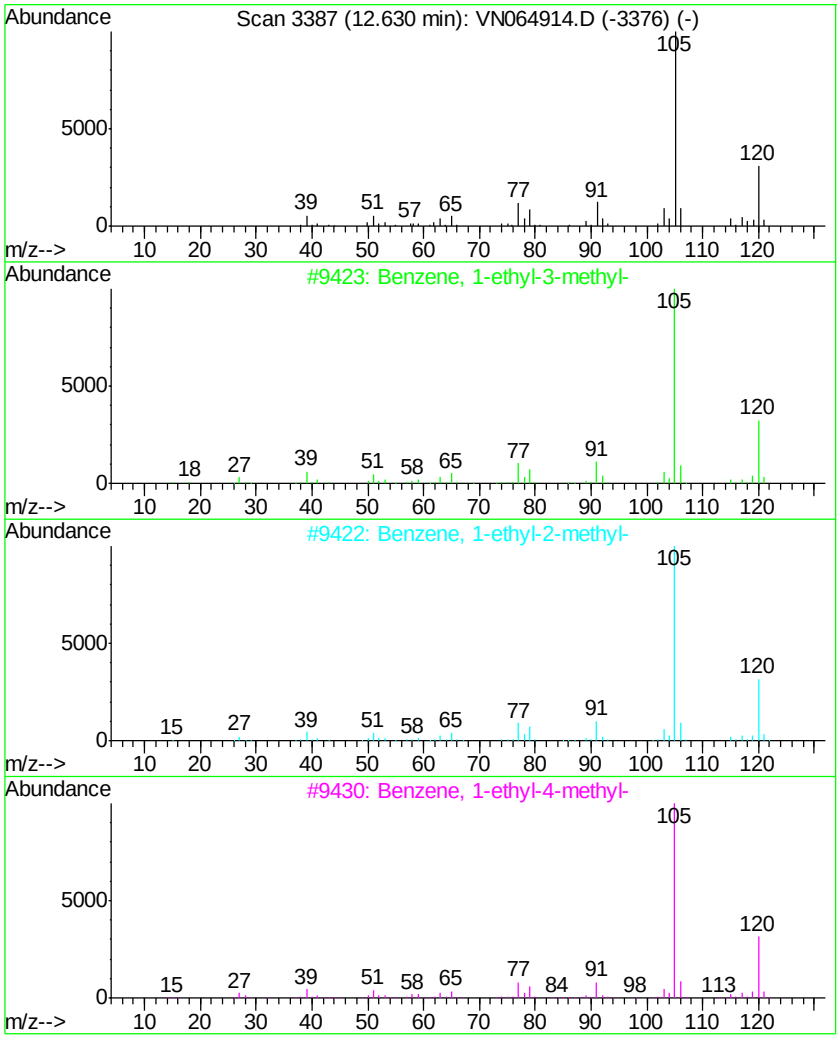
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

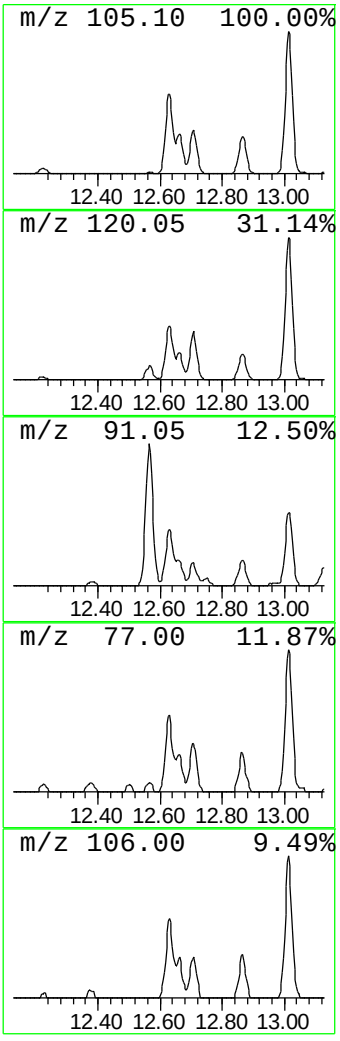
****

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.60 ug/l	142789	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
Data File : VN064914.D
Acq On : 4 Dec 2020 13:16
Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

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

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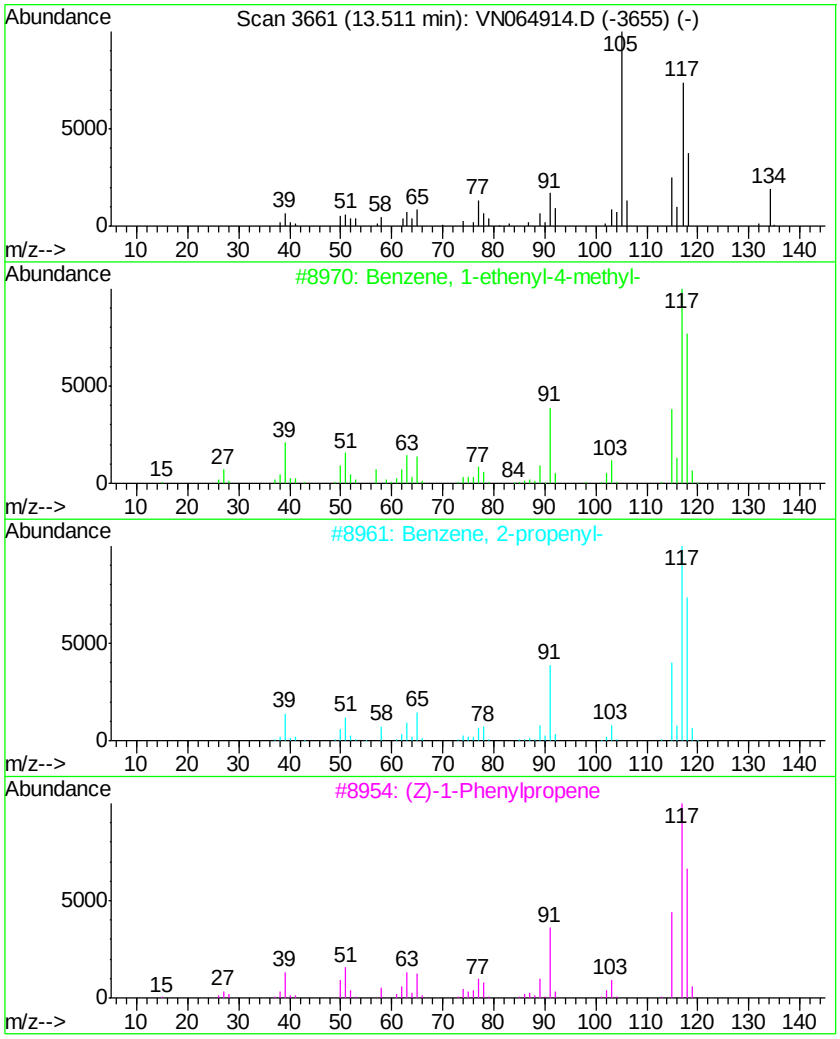
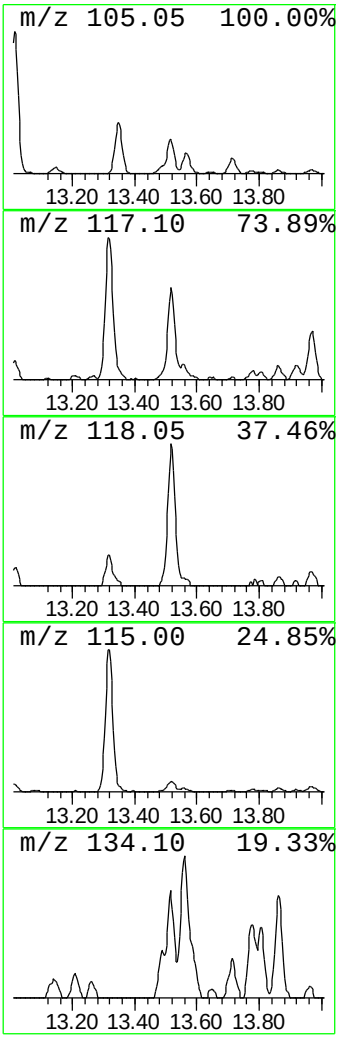
Peak Number 3 Benzene, 1-ethenyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	5.29 ug/l	99265	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	60
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	60
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	53
5	Indane	118	C9H10	000496-11-7	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
Data File : VN064914.D
Acq On : 4 Dec 2020 13:16
Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

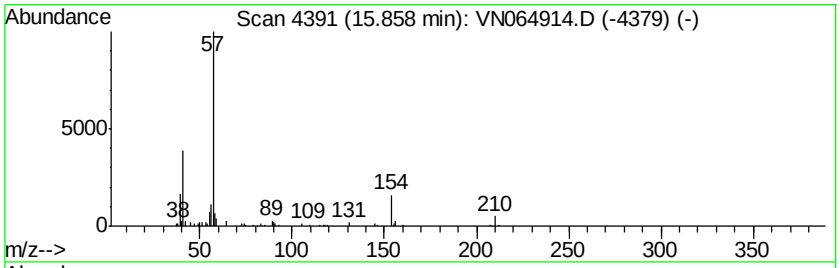
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

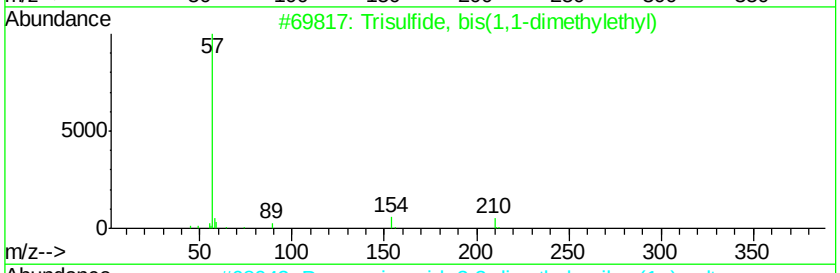
****

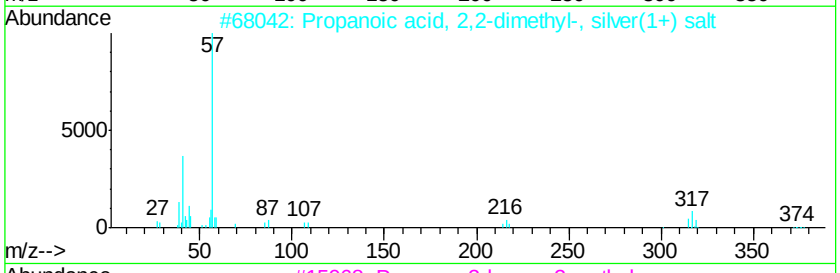
Peak Number 4 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

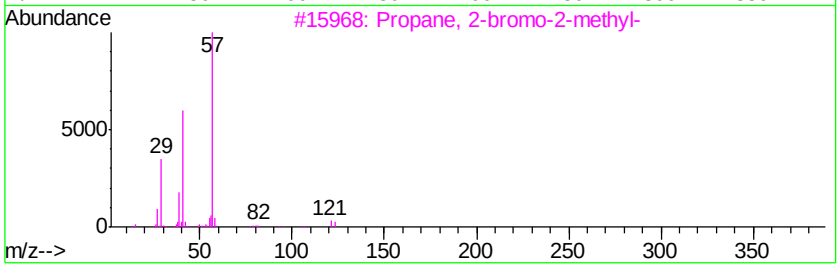
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	6.97 ug/l	130936	1,4-Dichlorobenzene-d4	13.32

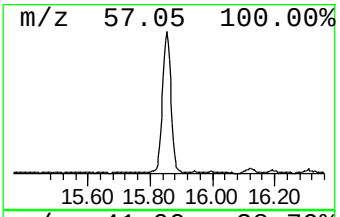
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	52
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	37
3	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	35
4	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	32
5	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	32

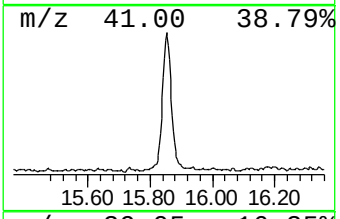


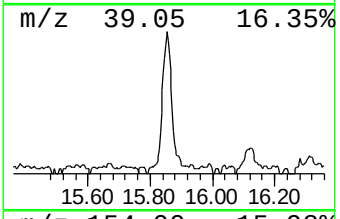


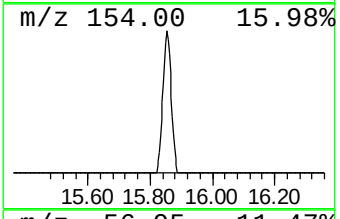


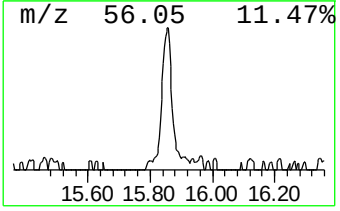












Library Search Compound Report

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Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

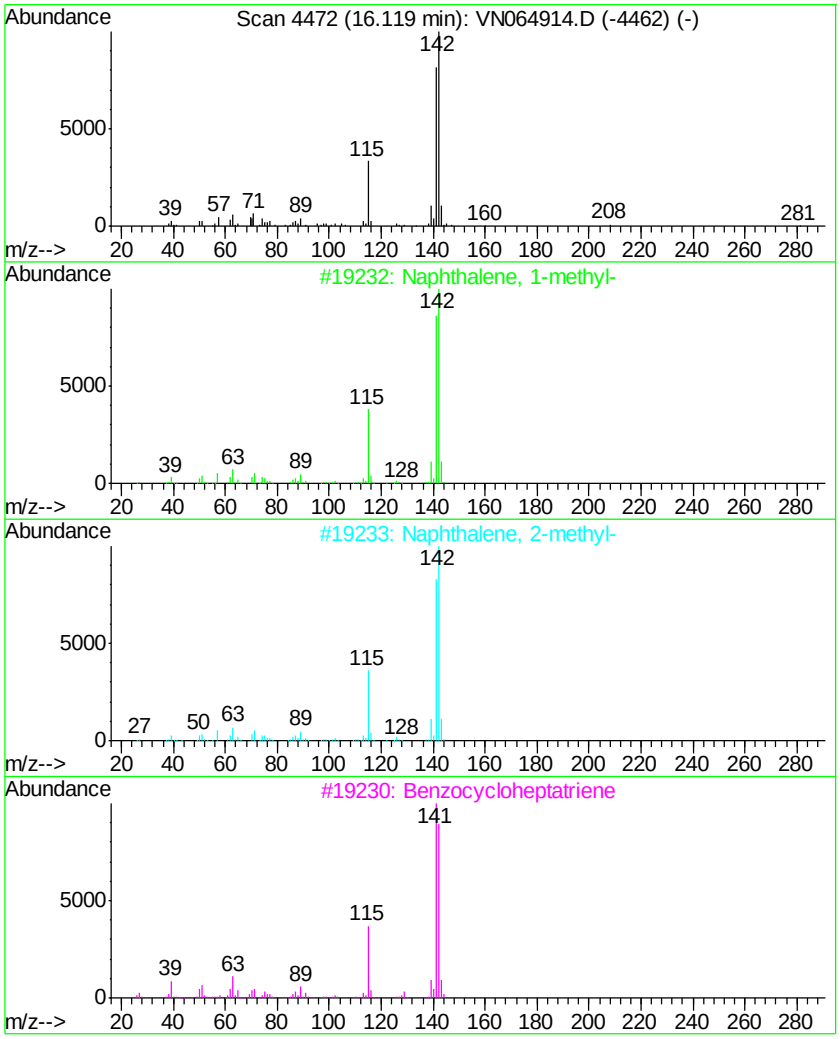
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

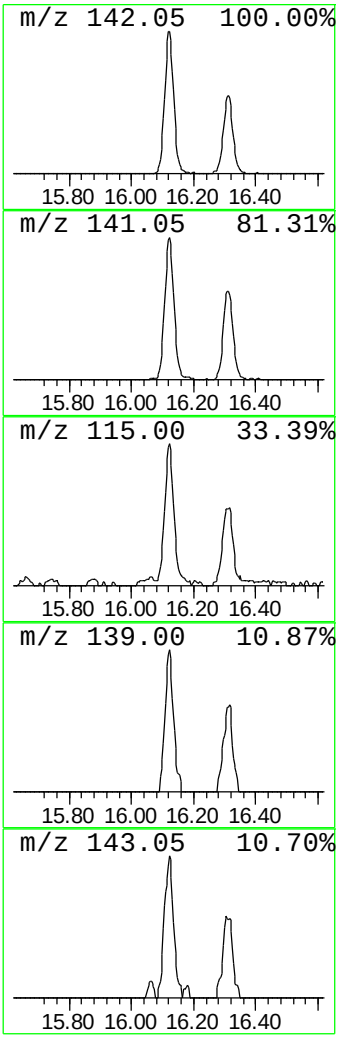
****

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	7.06 ug/l	132644	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	Naphthalene, 1-(2-hydroxypropyl)	186	C13H14O	027653-13-0	83
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	78





Library Search Compound Report

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Data File : VN064914.D
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Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

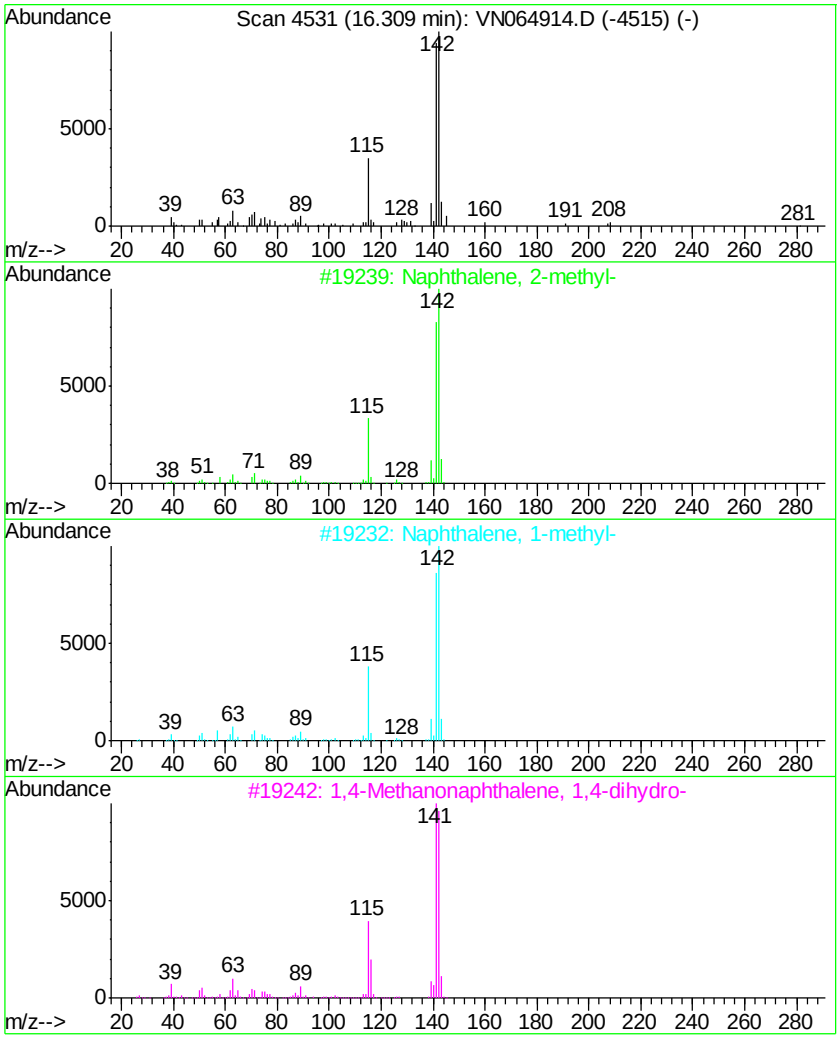
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

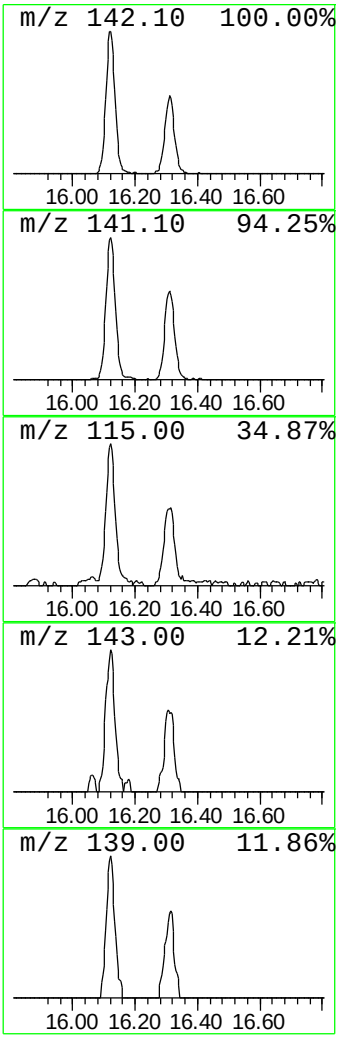
****

Peak Number 6 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	5.89 ug/l	110679	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120420\
Data File : VN064914.D
Acq On : 4 Dec 2020 13:16
Operator : JC/MD
Sample : L4918-05
Misc : 5.08G/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 16829

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.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
Hexane, 3-methyl-	7.83	5.3	ug/l	52996	1	7.62	498051	50.0
Benzene, 1-ethyl-...	12.63	7.6	ug/l	142789	4	13.32	938857	50.0
Benzene, 1-etheny...	13.51	5.3	ug/l	99265	4	13.32	938857	50.0
Trisulfide, bis(1...	15.86	7.0	ug/l	130936	4	13.32	938857	50.0
Naphthalene, 1-me...	16.12	7.1	ug/l	132644	4	13.32	938857	50.0
1,4-Methanonaphth...	16.31	5.9	ug/l	110679	4	13.32	938857	50.0