LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059333.D
Acq On : 21 Nov 2019 14:22
Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

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\82N112019W.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	2.452	192	211	226	rBV8	12680	43626	1.33%	0.109%
2	7.571	1784	1803	1814	rBV	211259	527212	16.06%	1.316%
3	7.644	1814	1826	1853	rVB	424542	1016110	30.95%	2.536%
4	8.008	1919	1939	1960	rBV	244332	565125	17.21%	1.410%
5	8.570	2096	2114	2138	rBV	604244	1256905	38.28%	3.137%
6	10.082	2570	2584	2614	rBV	936436	1718656	52.35%	4.289%
7	10.715	2770	2781	2790	rBV2	43005	70631	2.15%	0.176%
8	10.815	2800	2812	2824	rBV2	27000	57716	1.76%	0.144%
9	11.001	2859	2870	2881	rBV2	77793	140151	4.27%	0.350%
10	11.120	2894	2907	2915	rBV4	57723	110395	3.36%	0.275%
11	11.204	2915	2933	2948	rVB5	87789	263459	8.02%	0.657%
12	11.297	2950	2962	2982	rBV	100797	209686	6.39%	0.523%
13	11.403	2982	2995	3014	rBV	788312	1413518	43.05%	3.527%
14	11.541	3029	3038	3044	rBV2	49187	75690	2.31%	0.189%
15	11.596	3044	3055	3063	rBV6	87749	174087	5.30%	0.434%
16	11.654	3064	3073	3080	rBV2	168539	301803	9.19%	0.753%
17	11.696	3082	3086	3096	rVB3	152582	224318	6.83%	0.560%
18	11.757	3096	3105	3111	rBV2	65397	118774	3.62%	0.296%
19	11.799	3112	3118	3126	rBV3	25520	47325	1.44%	0.118%
20	11.853	3127	3135	3143	rBV3	148555	230905	7.03%	0.576%
21	11.927	3143	3158	3169	rBV8	458858	1150042	35.03%	2.870%
22	11.982	3170	3175	3180	rBV2	93180	110371	3.36%	0.275%
23	12.046	3186	3195	3204	rVB	1200281	1718782	52.35%	4.289%
24	12.120	3209	3218	3222	rBV3	443783	727589	22.16%	1.816%
25	12.156	3223	3229	3240	rVB3	853459	1474817	44.92%	3.680%
26	12.294	3262	3272	3281	rBV6	511375	958722	29.20%	2.393%
27	12.403	3294	3306	3317	rBV2	766618	1504240	45.82%	3.754%
28	12.493	3318	3334	3341	rBV6	345033	900044	27.41%	2.246%
29	12.561	3348	3355	3369	rVB2	1079231	2097983	63.90%	5.236%
30	12.647	3369	3382	3392	rBV5	580922	1444723	44.00%	3.605%
31	12.731	3394	3408	3416	rBV5	1279549	3283171	100.00%	8.193%
32	12.873	3445	3452	3459	rBV4	639991	966354	29.43%	2.412%
33	12.966	3475	3481	3493	rVB5	1008452	1844062	56.17%	4.602%
34	13.094	3513	3521	3530	rBV	790822	1289499	39.28%	3.218%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

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\82N112019W.M
Title : SW846 8260

35	13.146	3530	3537	3551	rVB5	944240	1811335	55.17%	4.520%
36	13.242	3552	3567	3575	rBV4	1300856	2962786	90.24%	7.394%
37	13.667	3689	3699	3708	rBV4	1475660	2819962	85.89%	7.037%
38	13.715	3710	3714	3722	rVB2	509967	652622	19.88%	1.629%
39	14.181	3848	3859	3885	rVB7	920342	2605405	79.36%	6.502%
40	14.336	3901	3907	3914	rVB4	330551	416155	12.68%	1.039%
41	14.596	3982	3988	3997	rVB3	227587	367426	11.19%	0.917%
42	14.651	3999	4005	4016	rVB4	228294	399367	12.16%	0.997%

Sum of corrected areas: 40071549

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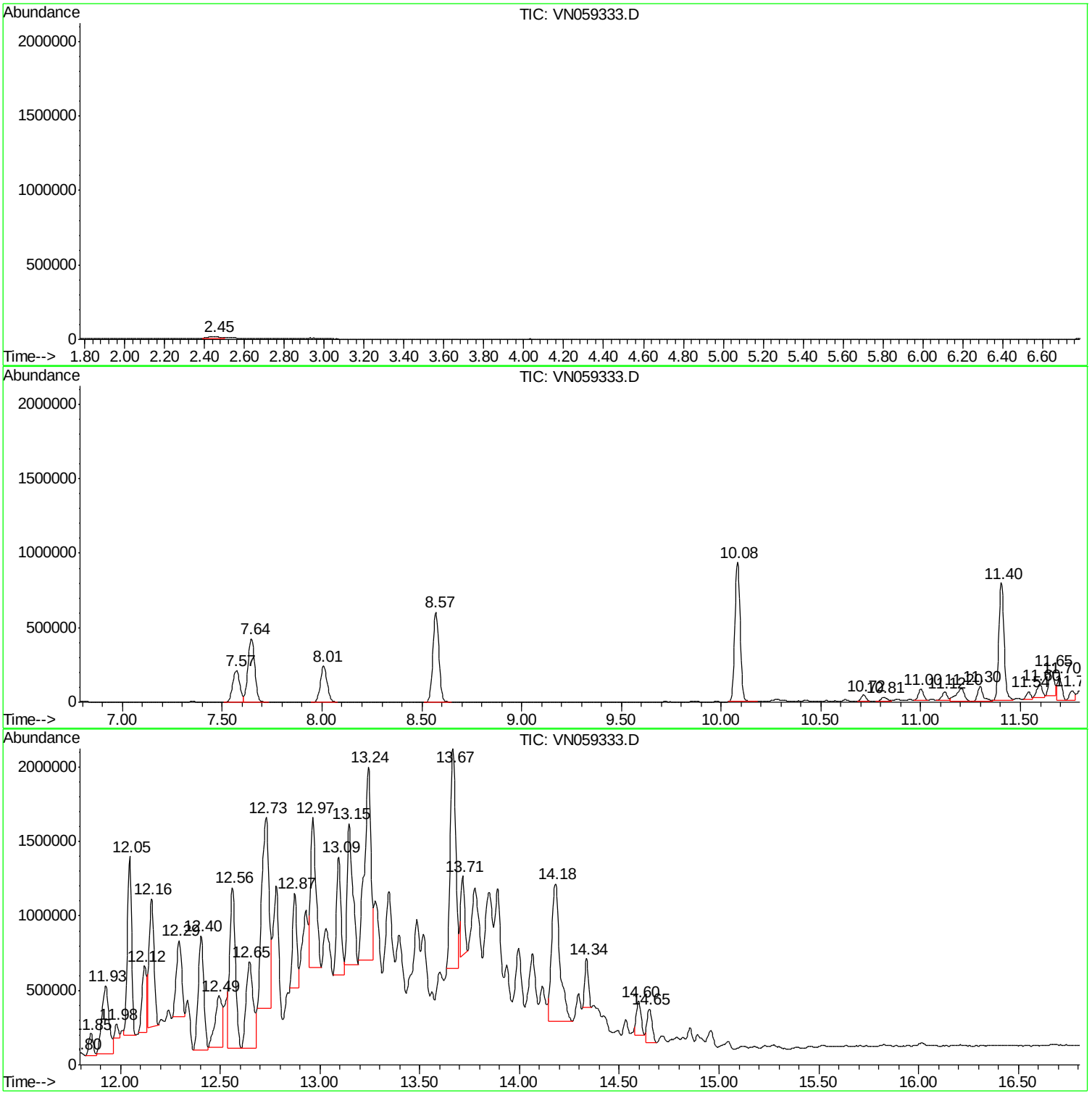
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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



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Data File : VN059333.D
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Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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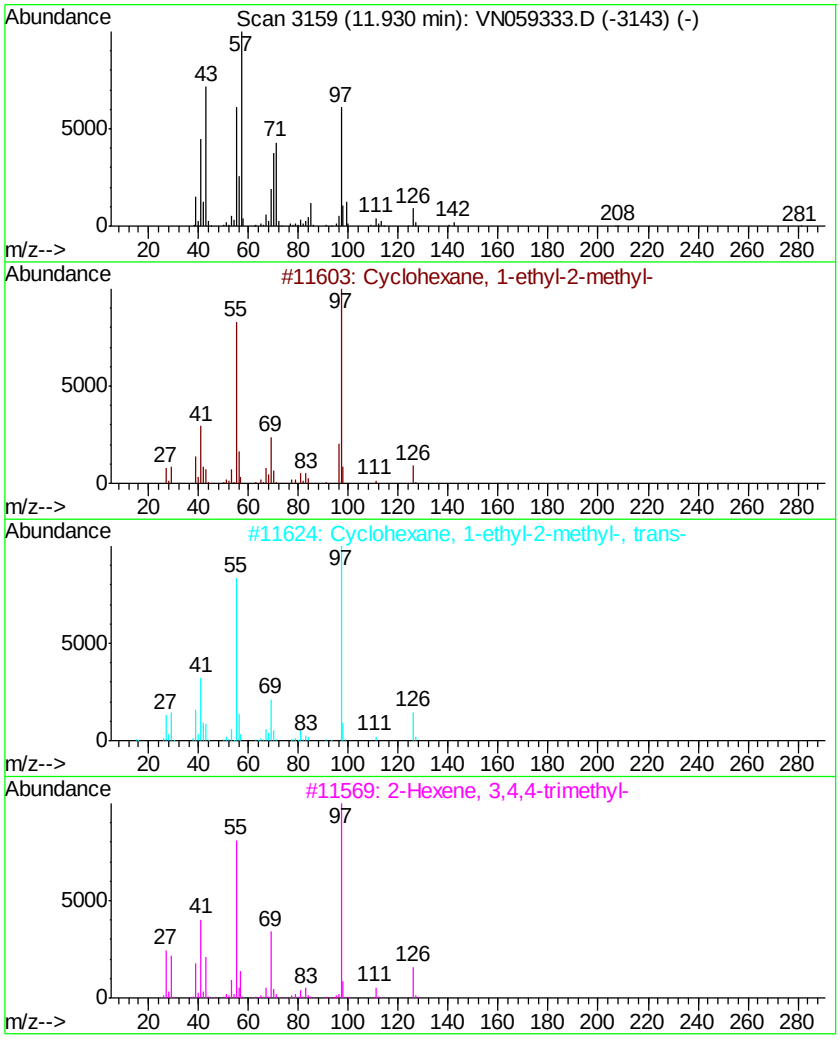
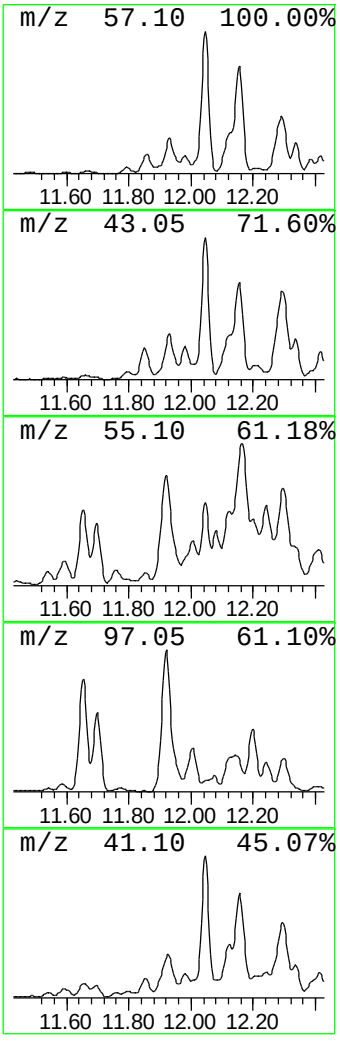
Peak Number 1 unknown11.93 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	40.68 ug/l	1150040	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	49
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	46
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	43
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	38
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	38





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Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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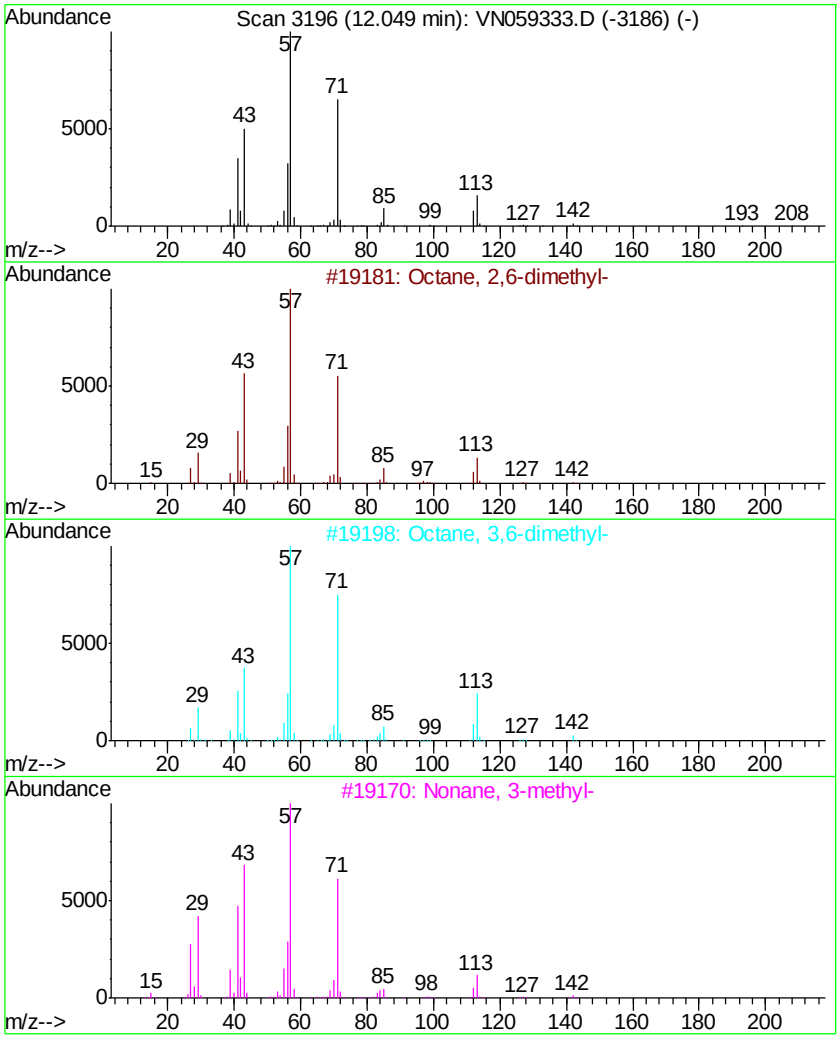
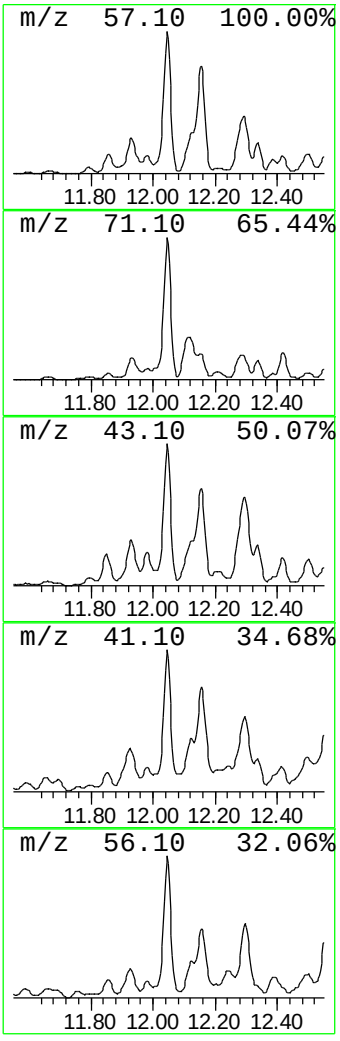
Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	60.80 ug/l	1718780	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	87
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	53





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Data File : VN059333.D
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Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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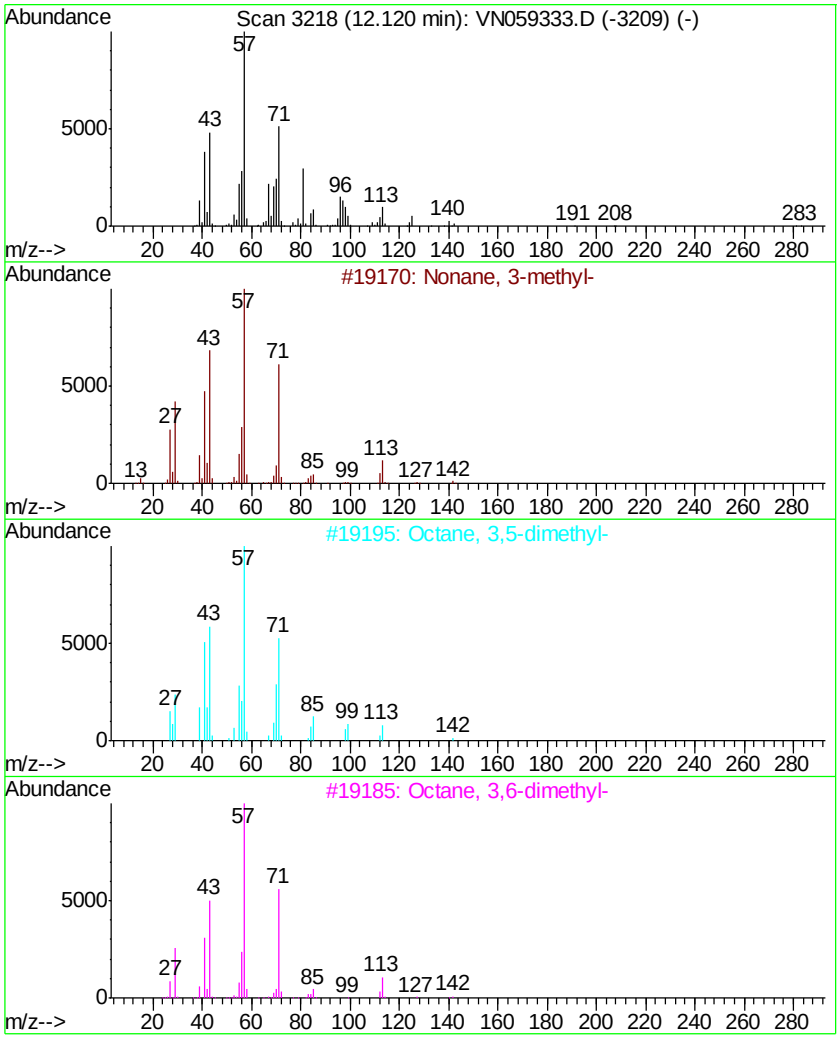
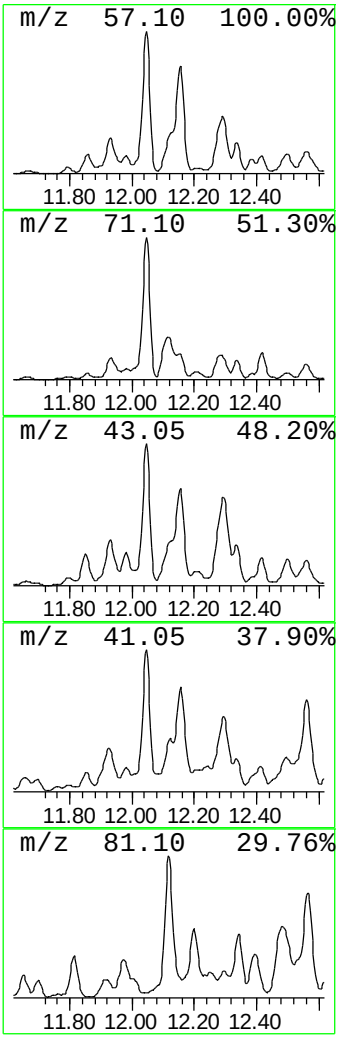
Peak Number 3 Nonane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	25.74 ug/l	727589	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	55
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	49
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	43
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059333.D
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Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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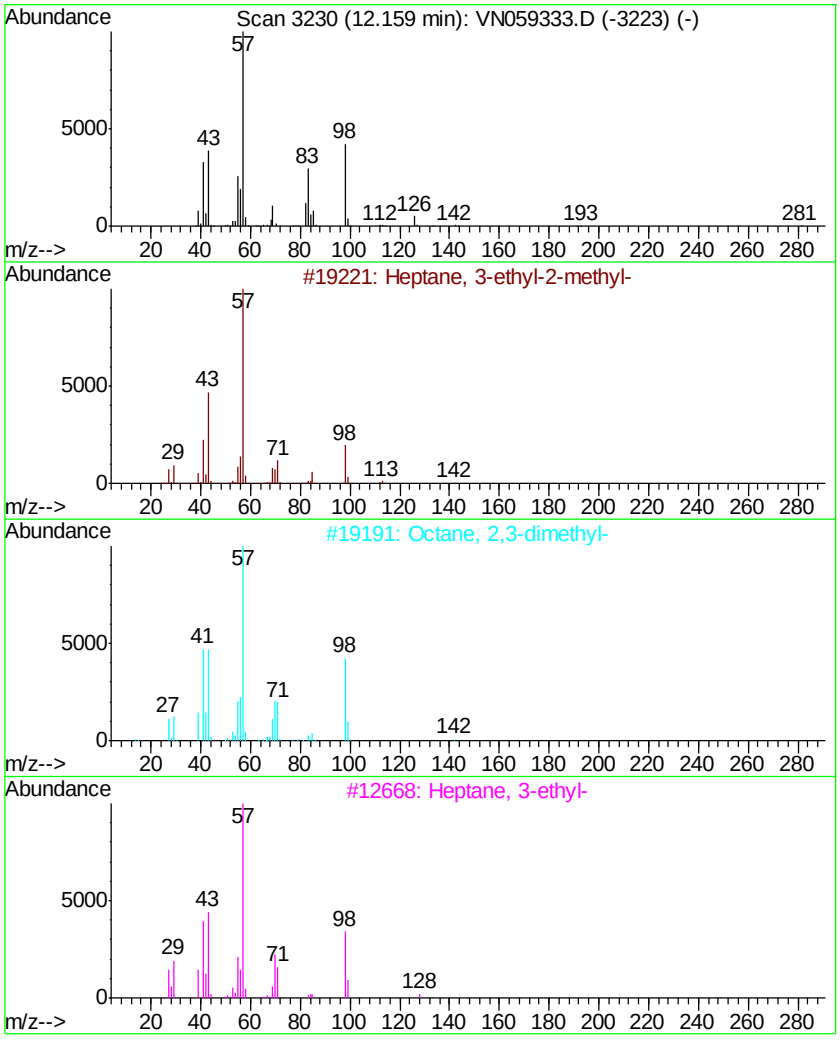
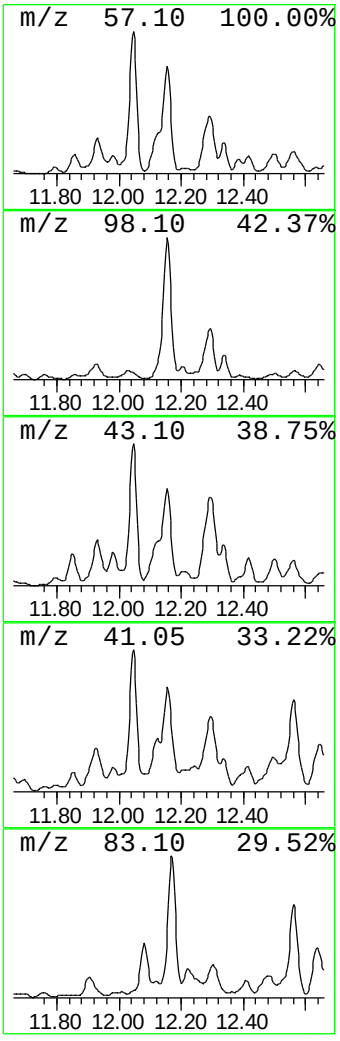
Peak Number 4 unknown12.16 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	52.17 ug/l	1474820	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	43
2	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	40
3	Heptane, 3-ethyl-	128	C9H20	015869-80-4	38
4	Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	35
5	1,3,2-Dioxaborolane, 4,4-dimethy...	142	C6H11BO3	1000063-89-2	33





Library Search Compound Report

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Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
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TIC Library : C:\DATABASE\NIST11.L
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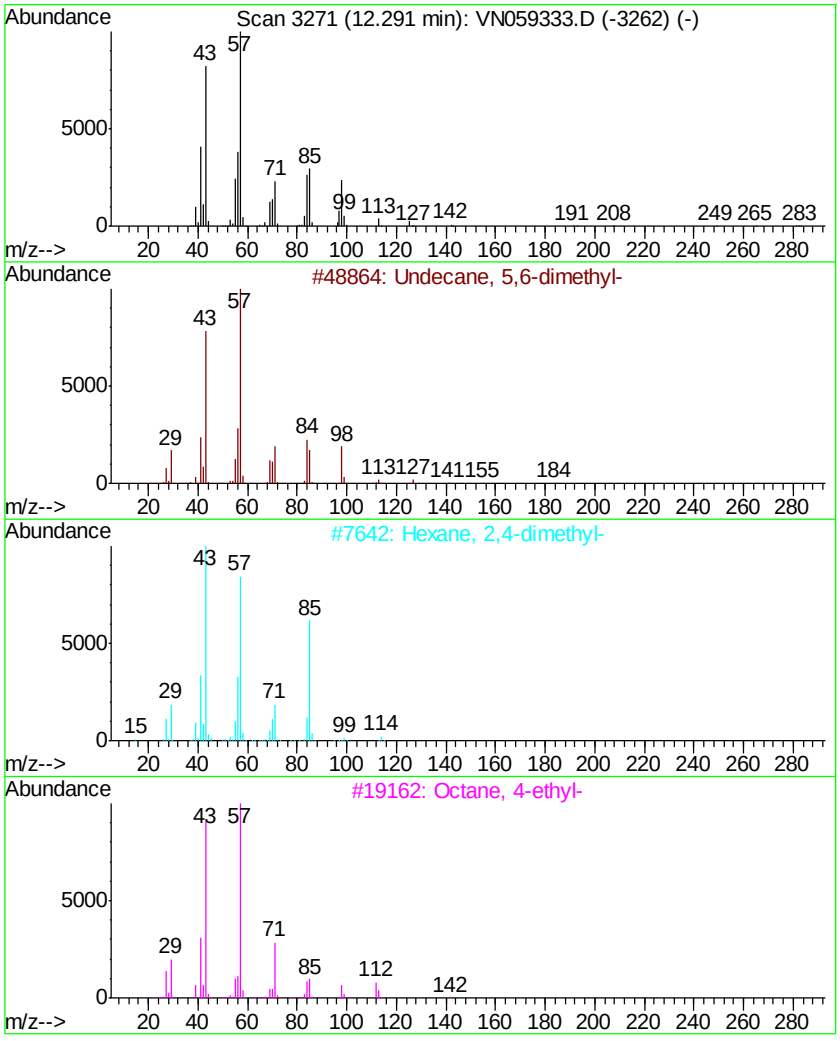
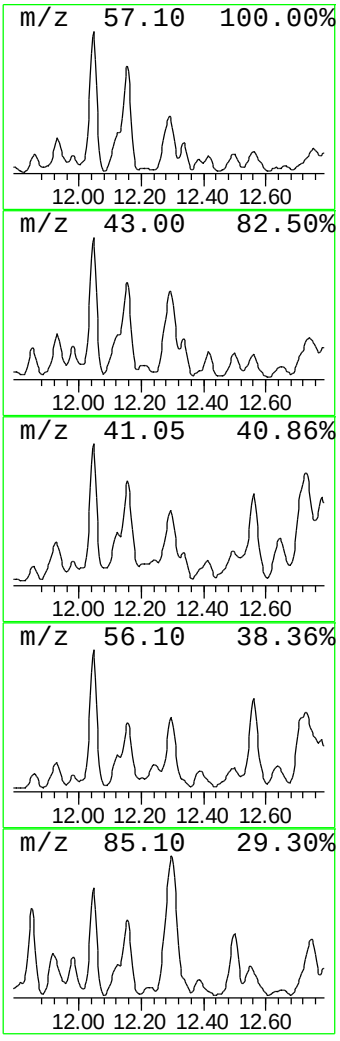
Peak Number 5 Undecane, 5,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	33.91 ug/l	958722	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5,6-dimethyl-	184	C13H28	017615-91-7	80
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	52
3	Octane, 4-ethyl-	142	C10H22	015869-86-0	50
4	Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	43
5	Heptane, 4-ethyl-	128	C9H20	002216-32-2	43





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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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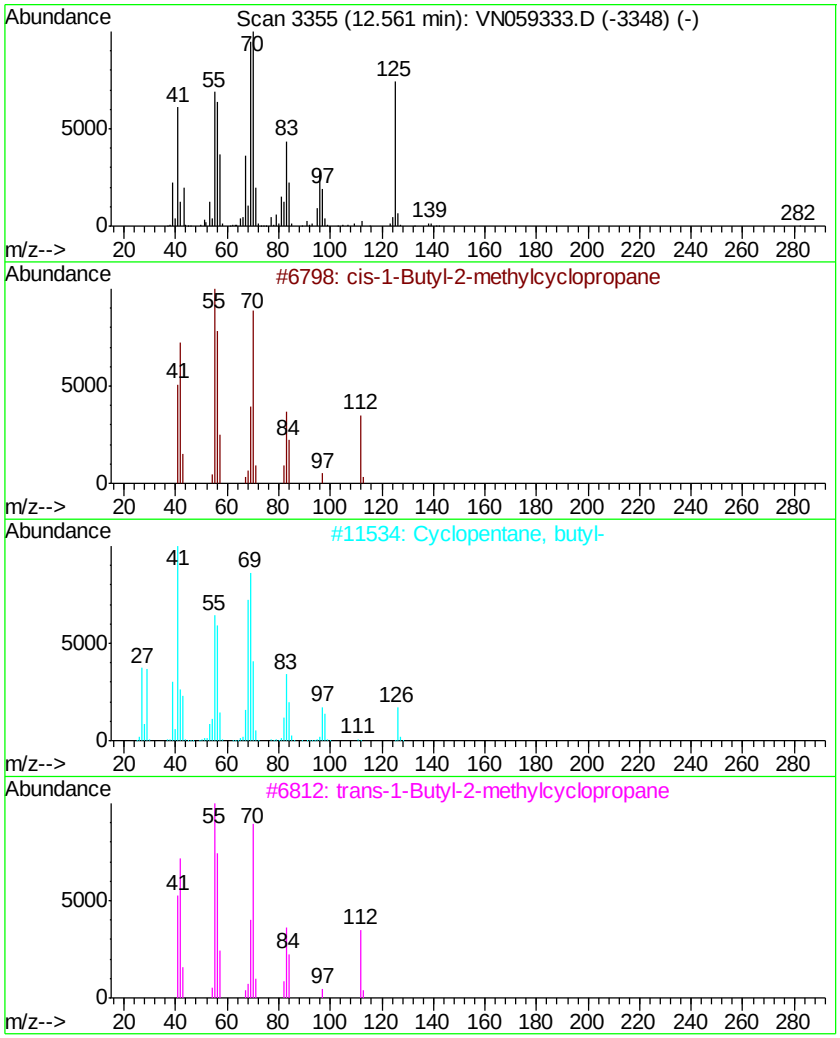
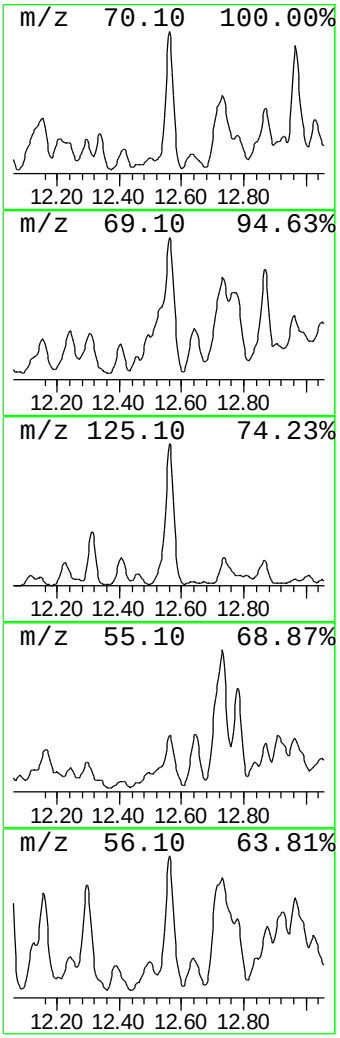
Peak Number 6 unknown12.56 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	35.41 ug/l	2097980	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	46
2	Cyclopentane, butyl-	126	C9H18	002040-95-1	46
3	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	45
4	Zinc, bis[2-(1,1-dimethylethyl)-...	314	C18H34Zn	074793-36-5	43
5	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	38





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Quant Title : SW846 8260

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

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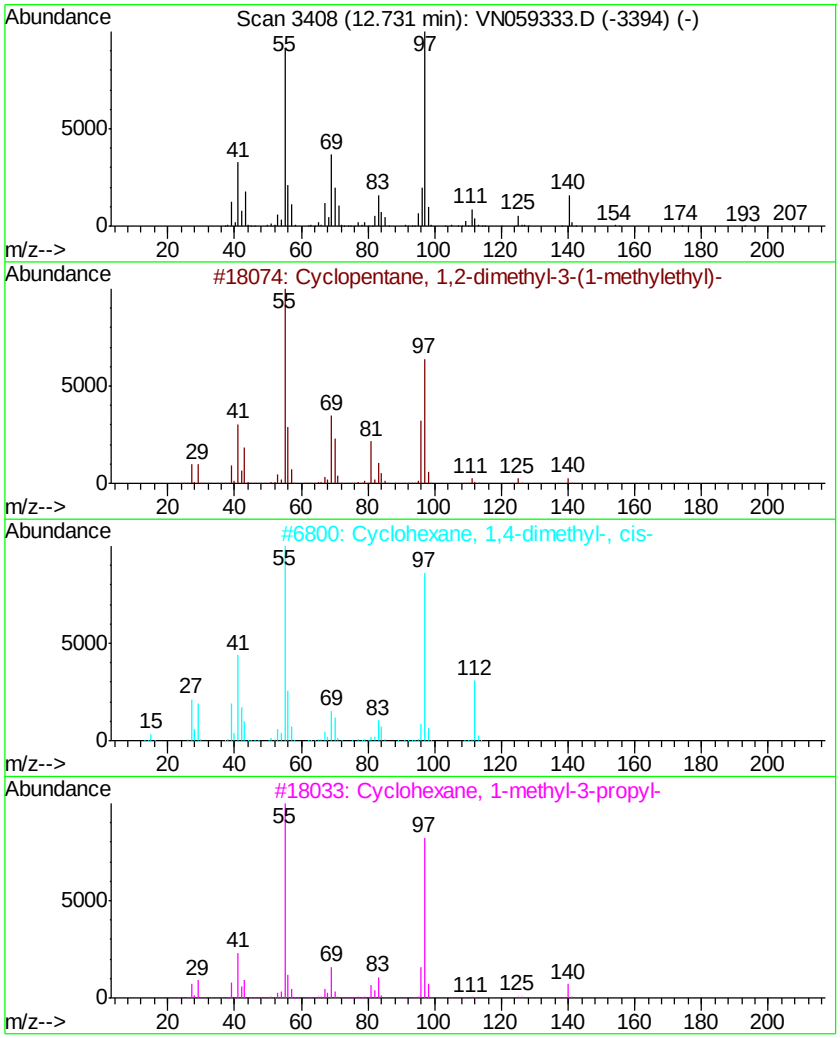
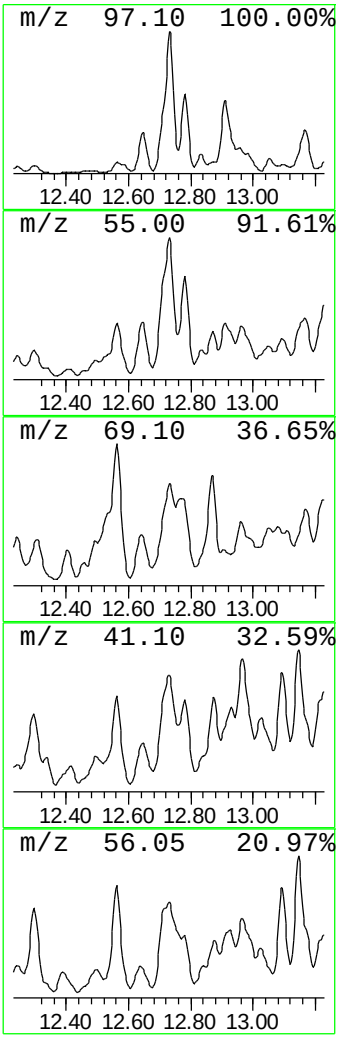
Peak Number 7 Cyclopentane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	55.41 ug/l	3283170	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-3-(1-...	140	C10H20	000489-20-3	80
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	59
3	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	58
4	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	58
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	52





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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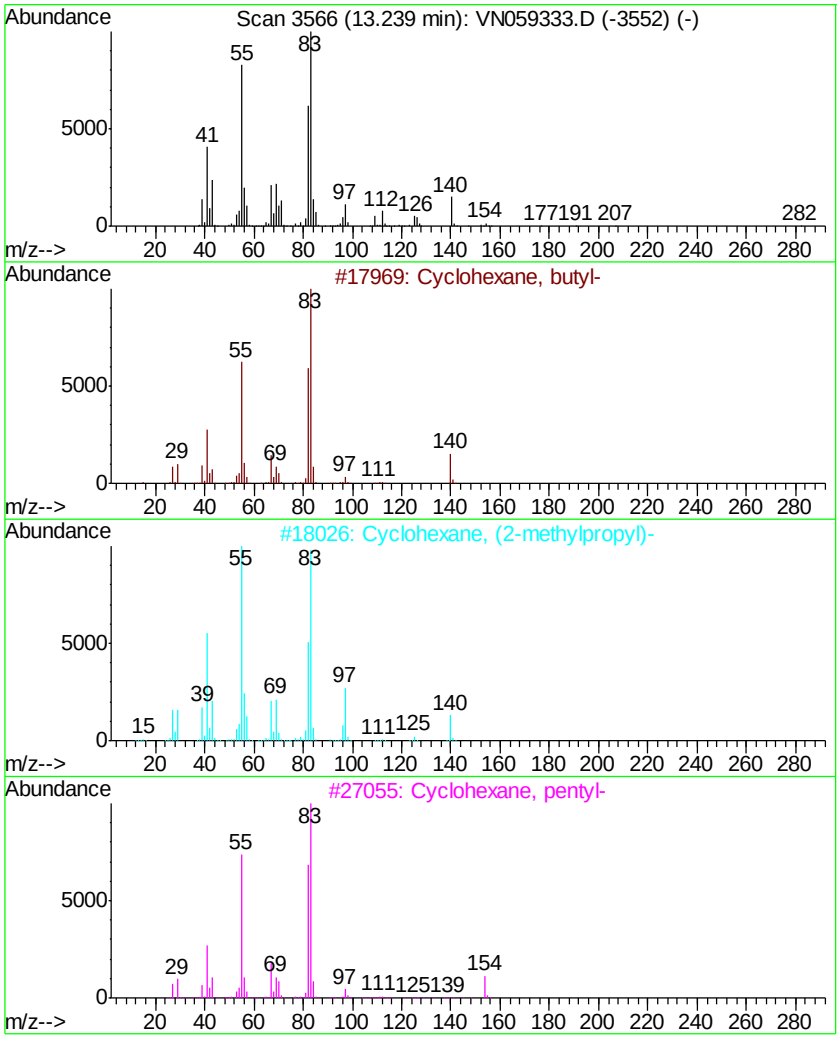
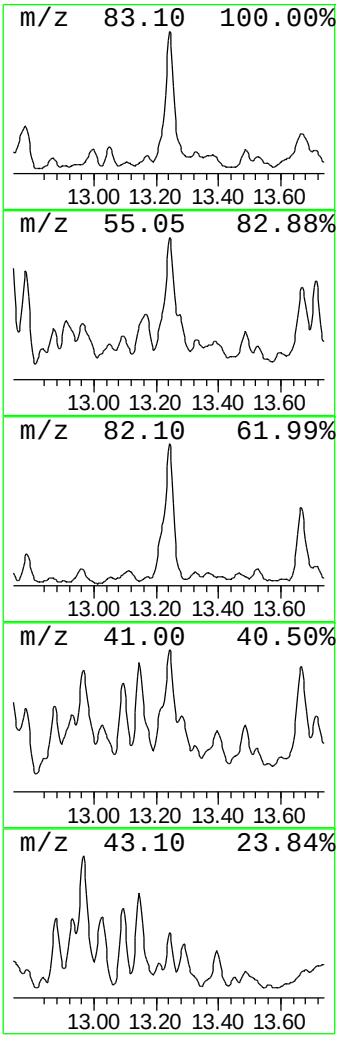
Peak Number 8 Cyclohexane, butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	50.00 ug/l	2962790	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	87
2	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	86
3	Cyclohexane, pentyl-	154	C11H22	004292-92-6	80
4	Cyclohexane, ethyl-	112	C8H16	001678-91-7	72
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059333.D
Acq On : 21 Nov 2019 14:22
Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

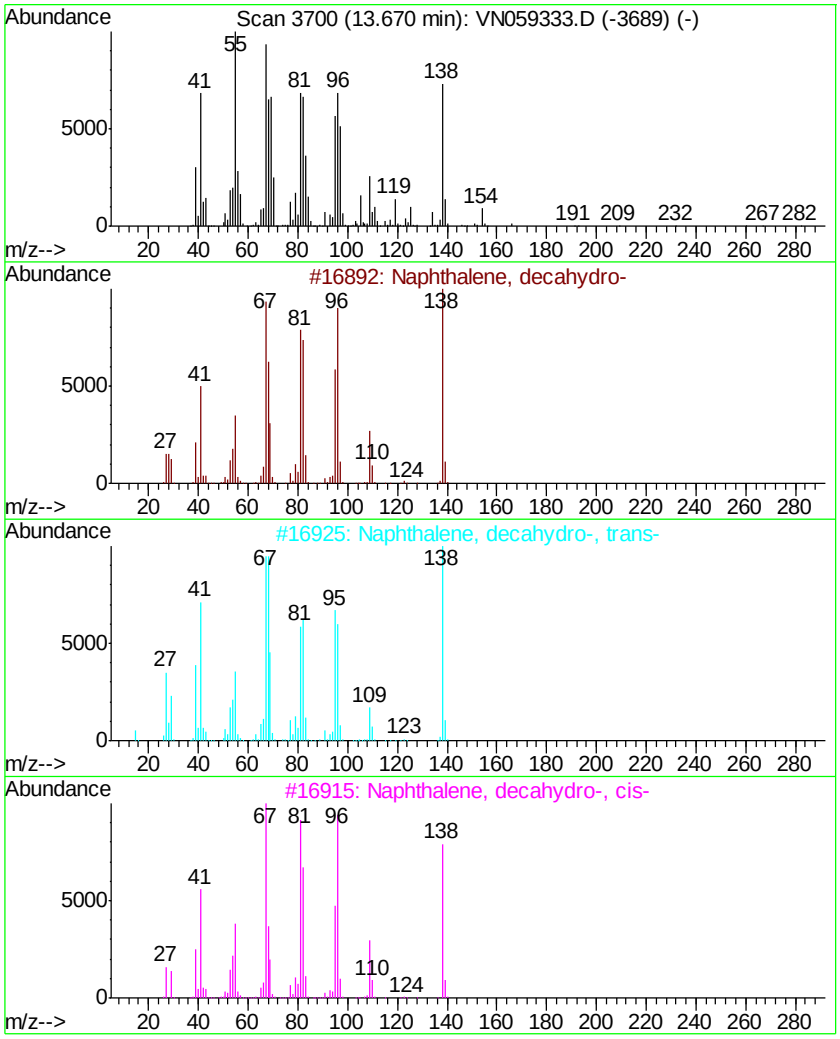
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

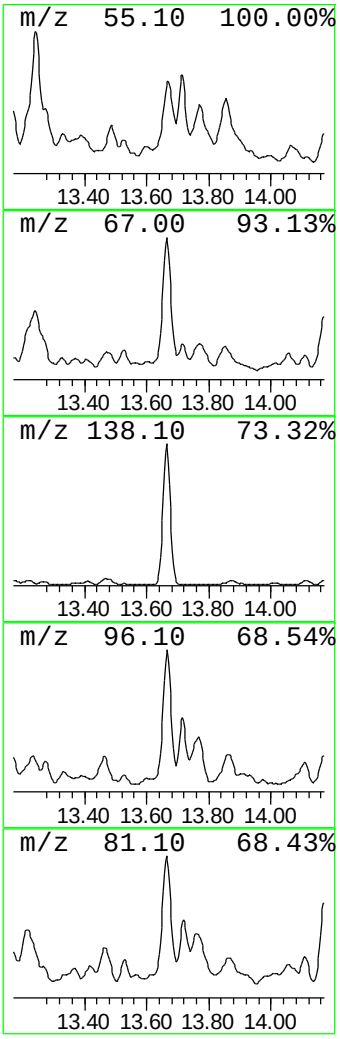
****

Peak Number 9 Naphthalene, decahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	47.59 ug/l	2819960	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	93
4	Spiro[4.5]decane	138	C10H18	000176-63-6	93
5	9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	70





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059333.D
Acq On : 21 Nov 2019 14:22
Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

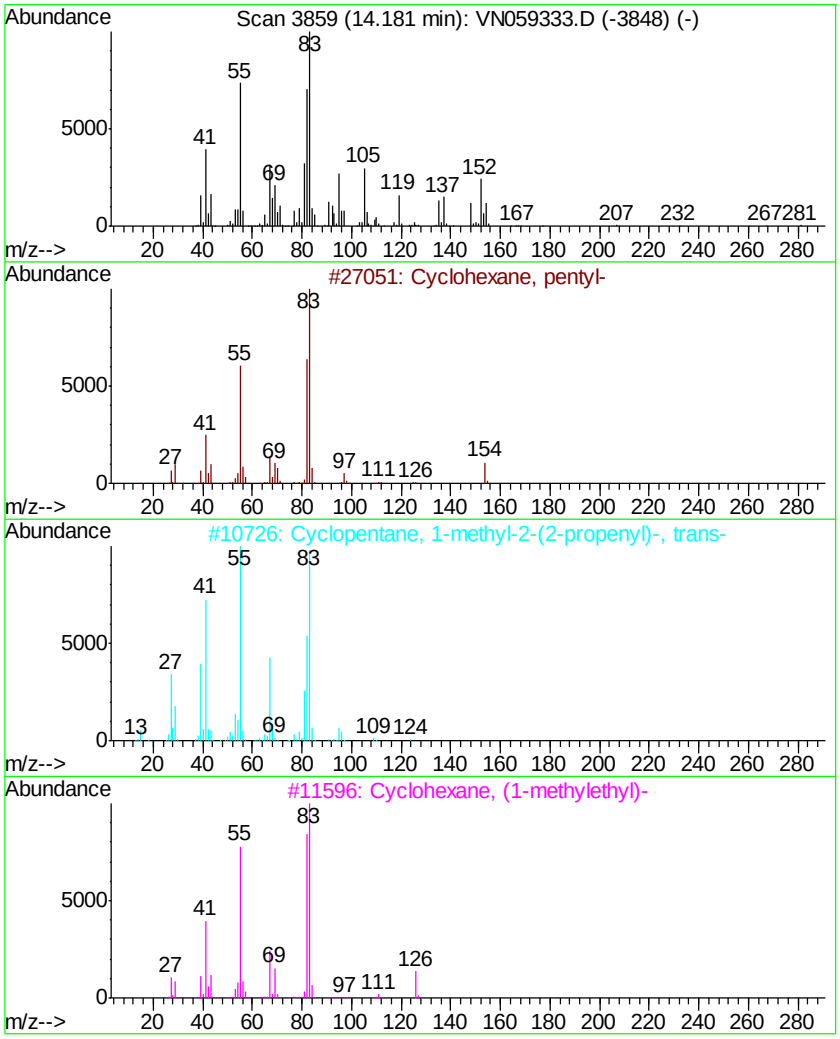
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

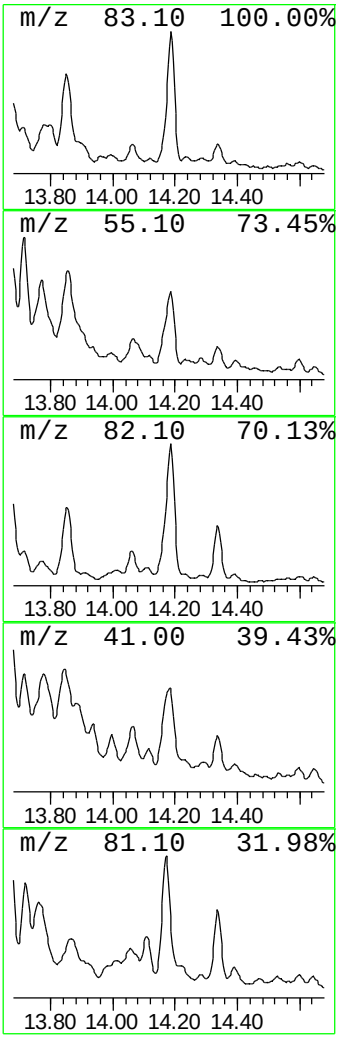
****

Peak Number 10 Cyclohexane, pentyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	43.97 ug/l	2605410	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	55
2	Cyclopentane, 1-methyl-2-(2-prop...	124	C9H16	050746-53-7	46
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	45
4	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	41
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059333.D
Acq On : 21 Nov 2019 14:22
Operator : JC/SP
Sample : K5957-07 10X
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.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
unknown11.93	11.93	40.7	ug/l	1150040	3	11.40	1413520	50.0
Octane, 2,6-dimet...	12.05	60.8	ug/l	1718780	3	11.40	1413520	50.0
Nonane, 3-methyl-	12.12	25.7	ug/l	727589	3	11.40	1413520	50.0
unknown12.16	12.16	52.2	ug/l	1474820	3	11.40	1413520	50.0
Undecane, 5,6-dim...	12.29	33.9	ug/l	958722	3	11.40	1413520	50.0
unknown12.56	12.56	35.4	ug/l	2097980	4	13.35	2962790	50.0
Cyclopentane, 1,2...	12.73	55.4	ug/l	3283170	4	13.35	2962790	50.0
Cyclohexane, butyl-	13.24	50.0	ug/l	2962790	4	13.35	2962790	50.0
Naphthalene, deca...	13.67	47.6	ug/l	2819960	4	13.35	2962790	50.0
Cyclohexane, pentyl-	14.18	44.0	ug/l	2605410	4	13.35	2962790	50.0