LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

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\82N100418W.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	7.593	1789	1810	1821	rBV	573424	1441078	10.86%	1.218%
2	7.667	1821	1833	1852	rVB	925592	2169050	16.35%	1.834%
3	8.027	1925	1945	1969	rBV	537212	1256209	9.47%	1.062%
4	8.278	1987	2023	2026	rBV2	47299	196754	1.48%	0.166%
5	8.587	2104	2119	2139	rBV	1201872	2491659	18.78%	2.107%
6	10.091	2572	2587	2619	rBV	2239046	4194382	31.61%	3.546%
7	10.432	2685	2693	2706	rVB2	175752	325942	2.46%	0.276%
8	10.718	2771	2782	2796	rVB	383643	647565	4.88%	0.547%
9	10.821	2797	2814	2827	rBV	252960	553398	4.17%	0.468%
10	10.889	2827	2835	2849	rVV2	107406	206781	1.56%	0.175%
11	11.005	2861	2871	2880	rBV5	228047	429189	3.23%	0.363%
12	11.059	2881	2888	2897	rVV2	178341	278402	2.10%	0.235%
13	11.124	2898	2908	2916	rVV4	131847	225034	1.70%	0.190%
14	11.214	2926	2936	2952	rVB	992473	1780028	13.41%	1.505%
15	11.336	2966	2974	2982	rBV5	81907	133943	1.01%	0.113%
16	11.406	2983	2996	3014	rBV	1750216	3351230	25.25%	2.833%
17	11.542	3028	3038	3047	rBV2	577340	963817	7.26%	0.815%
18	11.599	3047	3056	3064	rBV3	413919	747293	5.63%	0.632%
19	11.664	3065	3076	3096	rVB7	735306	2557357	19.27%	2.162%
20	11.760	3096	3106	3111	rBV3	384621	699358	5.27%	0.591%
21	11.812	3113	3122	3128	rBV3	287310	510596	3.85%	0.432%
22	11.853	3128	3135	3142	rVB3	535768	774155	5.83%	0.655%
23	11.924	3142	3157	3168	rBV5	3126772	7371534	55.55%	6.232%
24	11.979	3170	3174	3179	rVV2	397933	407720	3.07%	0.345%
25	12.046	3186	3195	3203	rBV	4664672	6457770	48.66%	5.460%
26	12.120	3210	3218	3223	rBV3	2027909	3414431	25.73%	2.887%
27	12.152	3224	3228	3238	rVB2	2925492	4258472	32.09%	3.600%
28	12.403	3295	3306	3316	rBV3	2408230	4252549	32.05%	3.595%
29	12.493	3316	3334	3340	rBV8	1746665	4654104	35.07%	3.935%
30	12.561	3349	3355	3370	rVB5	4870828	9147909	68.93%	7.734%
31	12.648	3370	3382	3392	rBV8	2646683	6394272	48.18%	5.406%
32	12.718	3394	3404	3415	rBV8	2667384	6836796	51.52%	5.780%
33	12.869	3445	3451	3458	rVB6	1391393	1818664	13.70%	1.538%
34	12.963	3473	3480	3492	rVB	8104517	13270410	100.00%	11.219%

LSC Area Percent Report

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Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

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\82N100418W.M
Title : SW846 8260

35	13.091	3513	3520	3530	rBV4	1788477	2756567	20.77%	2.331%
36	13.146	3532	3537	3541	rBV3	1210717	1637551	12.34%	1.384%
37	13.214	3552	3558	3562	rBV5	1613128	2327528	17.54%	1.968%
38	13.660	3688	3697	3708	rBV2	5212476	9229551	69.55%	7.803%
39	14.172	3848	3856	3866	rBV7	1893377	3659403	27.58%	3.094%
40	14.332	3899	3906	3914	rVB4	1290621	1797619	13.55%	1.520%
41	14.529	3962	3967	3975	rVV4	260426	331247	2.50%	0.280%
42	14.590	3979	3986	3995	rVV7	532835	1040801	7.84%	0.880%
43	14.644	3996	4003	4015	rVB5	724114	1282821	9.67%	1.085%

Sum of corrected areas: 118280939

LSC Report - Integrated Chromatogram

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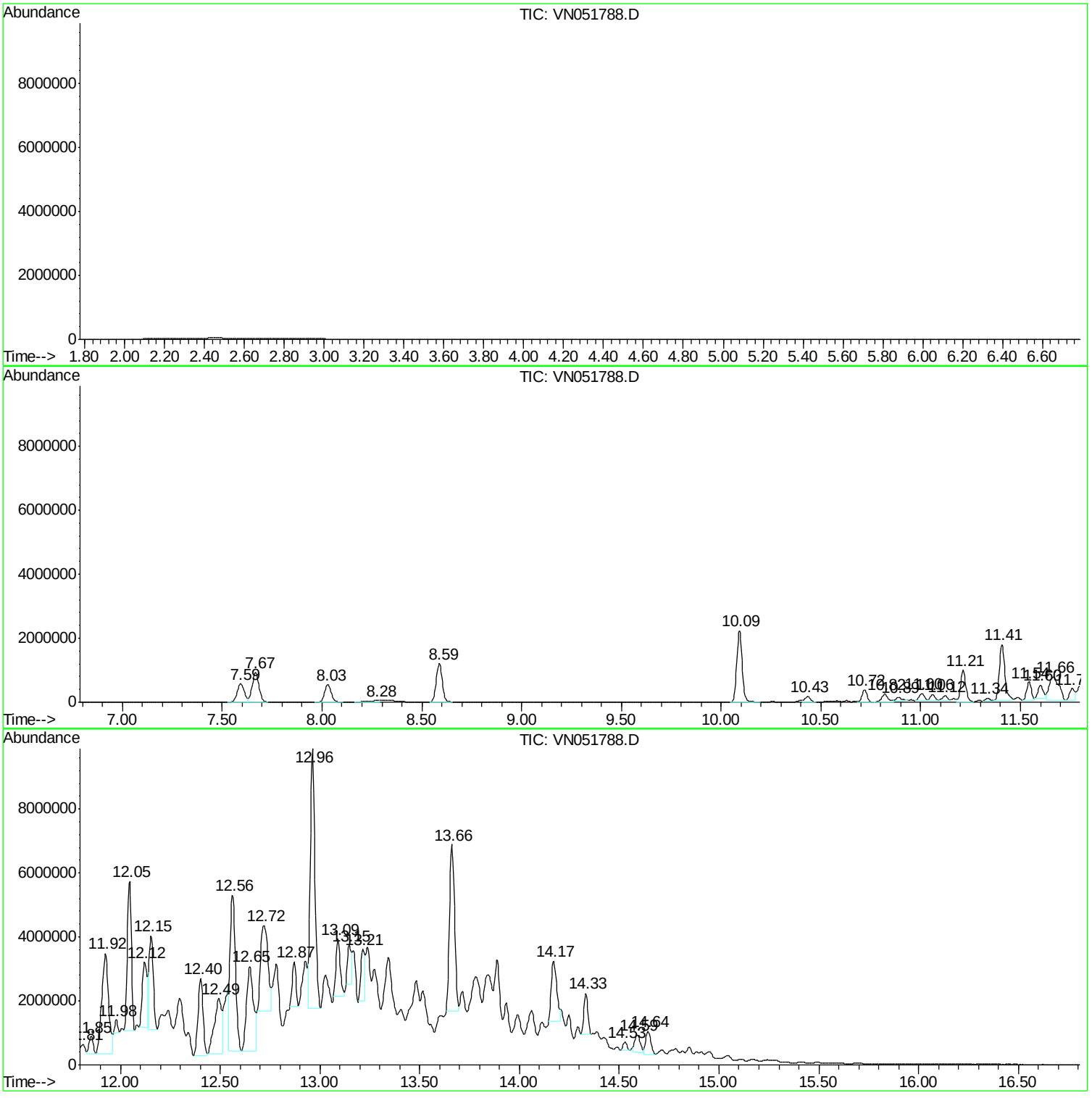
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
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Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

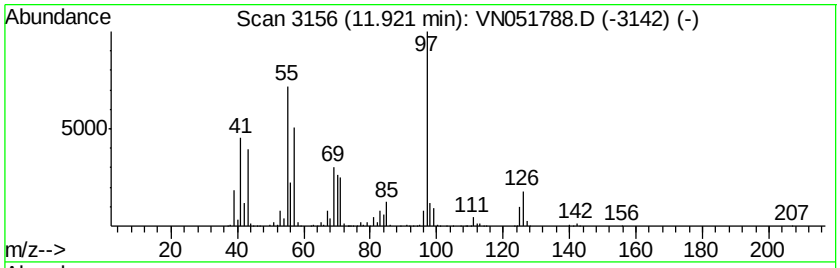
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

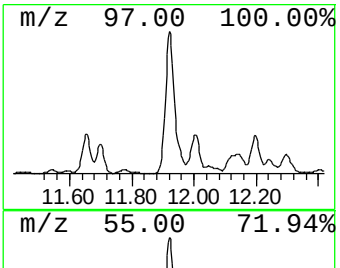
****

Peak Number 1 unknown11.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	109.98 ug/l	7371530	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	47
3	Thiophene, 2-propyl-	126	C7H10S	001551-27-5	47
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	47
5	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	46





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

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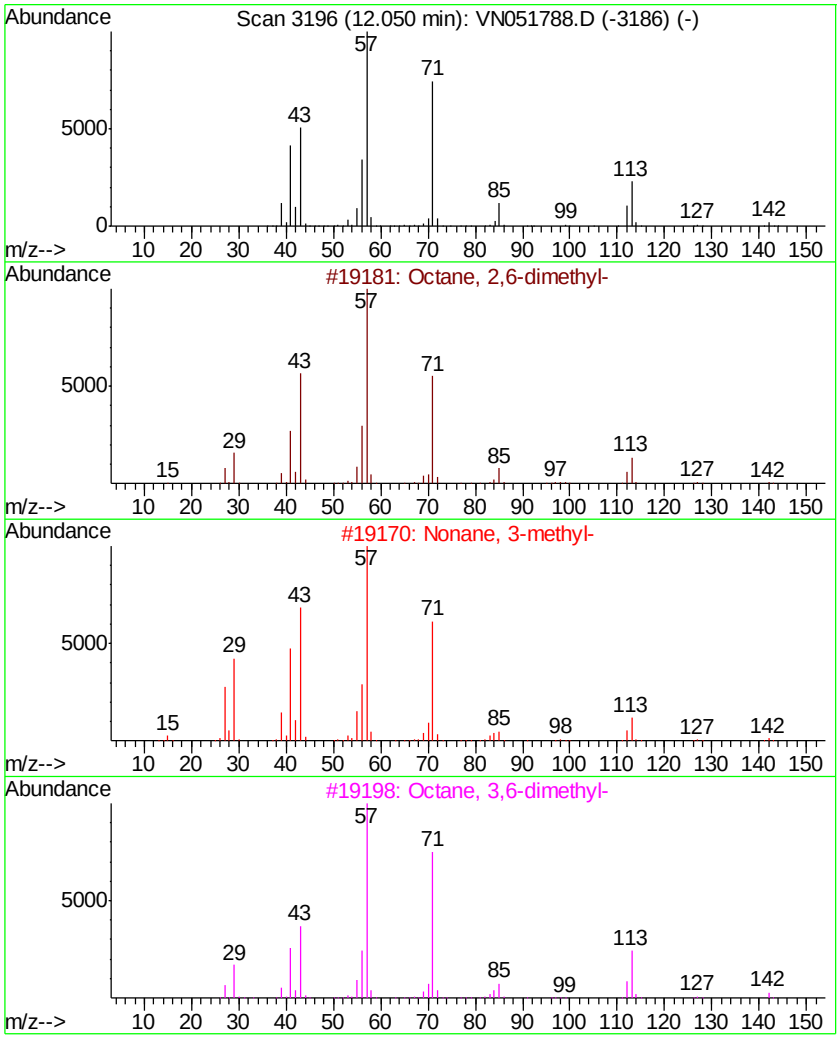
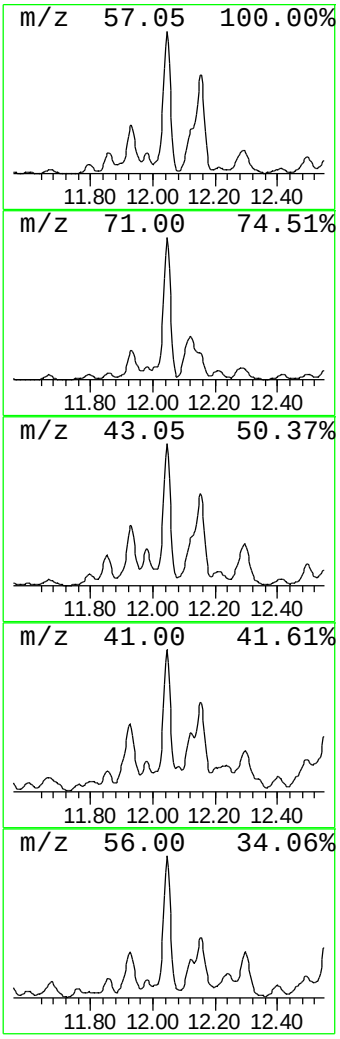
Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	96.35 ug/l	6457770	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
4	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

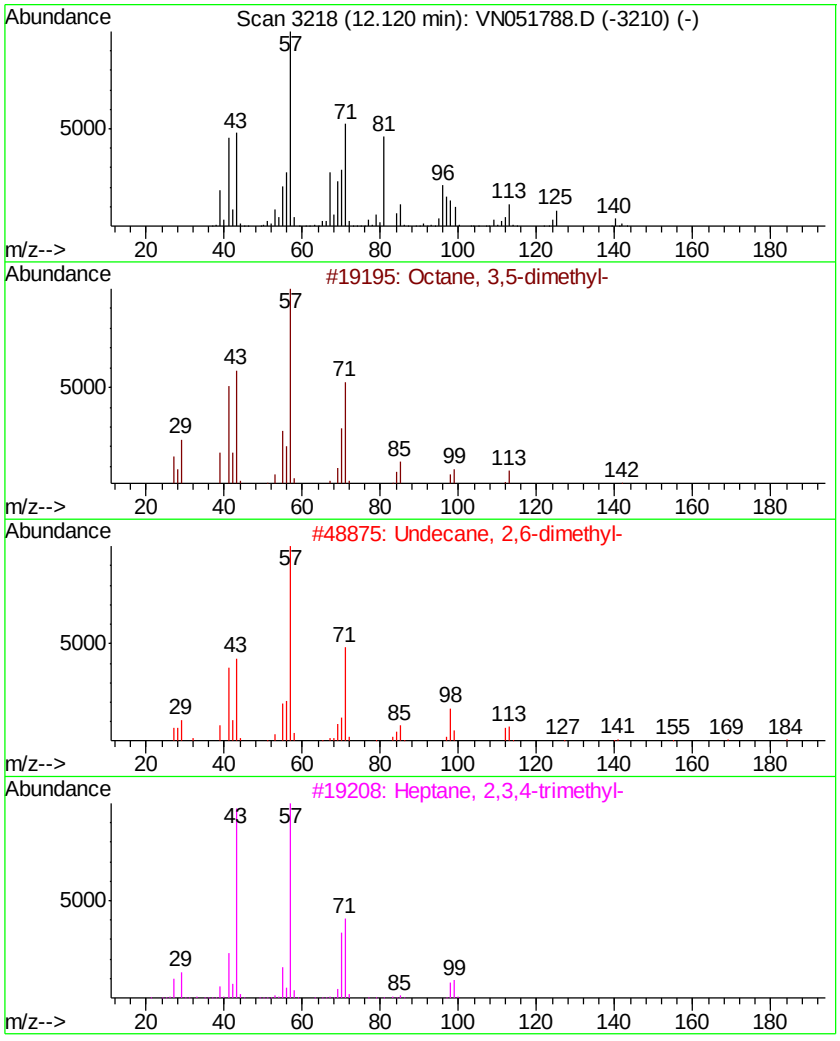
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

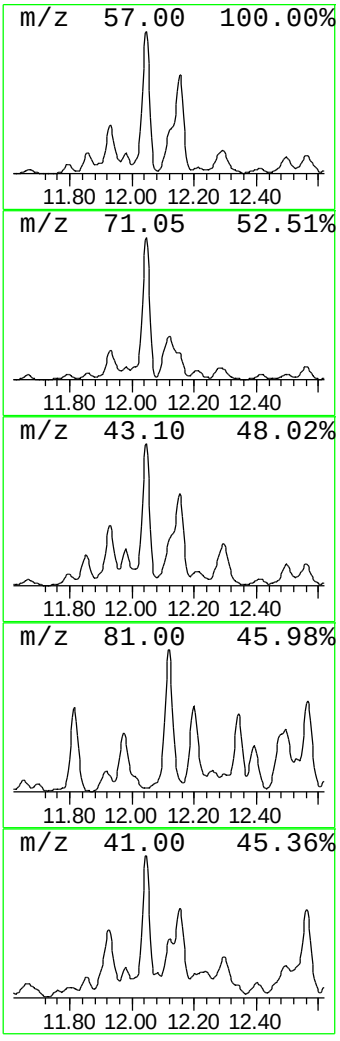
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octane, 3,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	50.94 ug/l	3414430	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	47
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	47
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	46
5	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

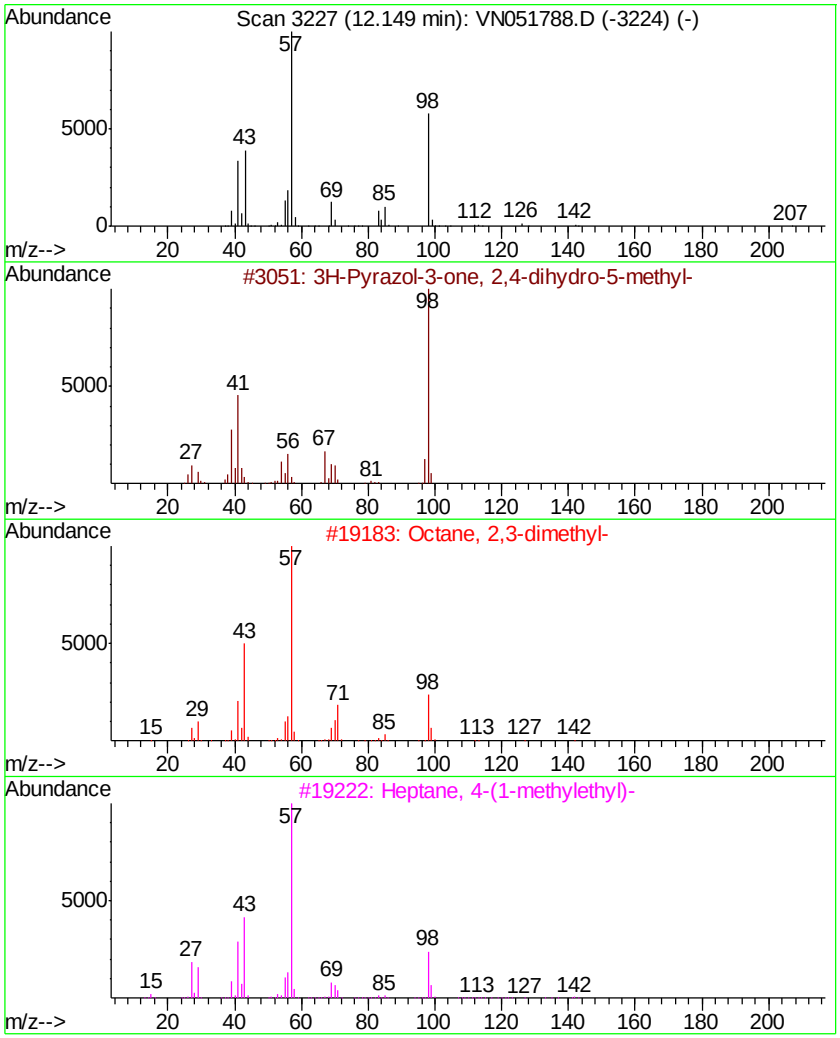
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

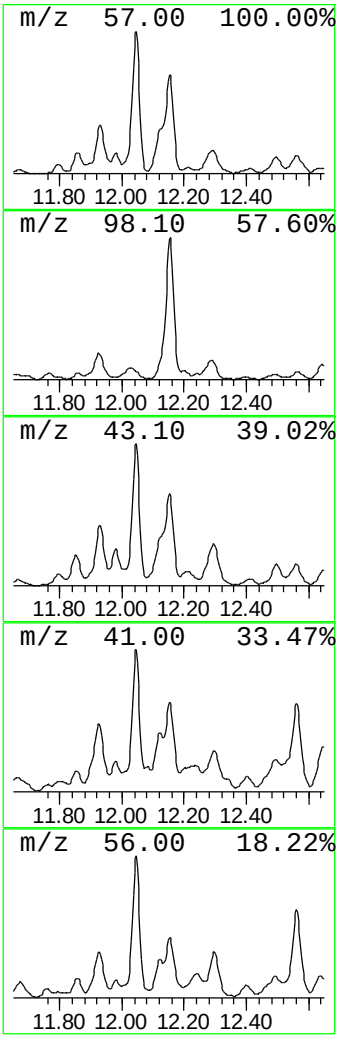
****

Peak Number 4 unknown12.15 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	63.54 ug/l	4258470	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	47
2	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	43
4	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	42
5	Cyclohexanone, 2-(1-methylethyl)-	140	C9H16O	001004-77-9	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
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Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

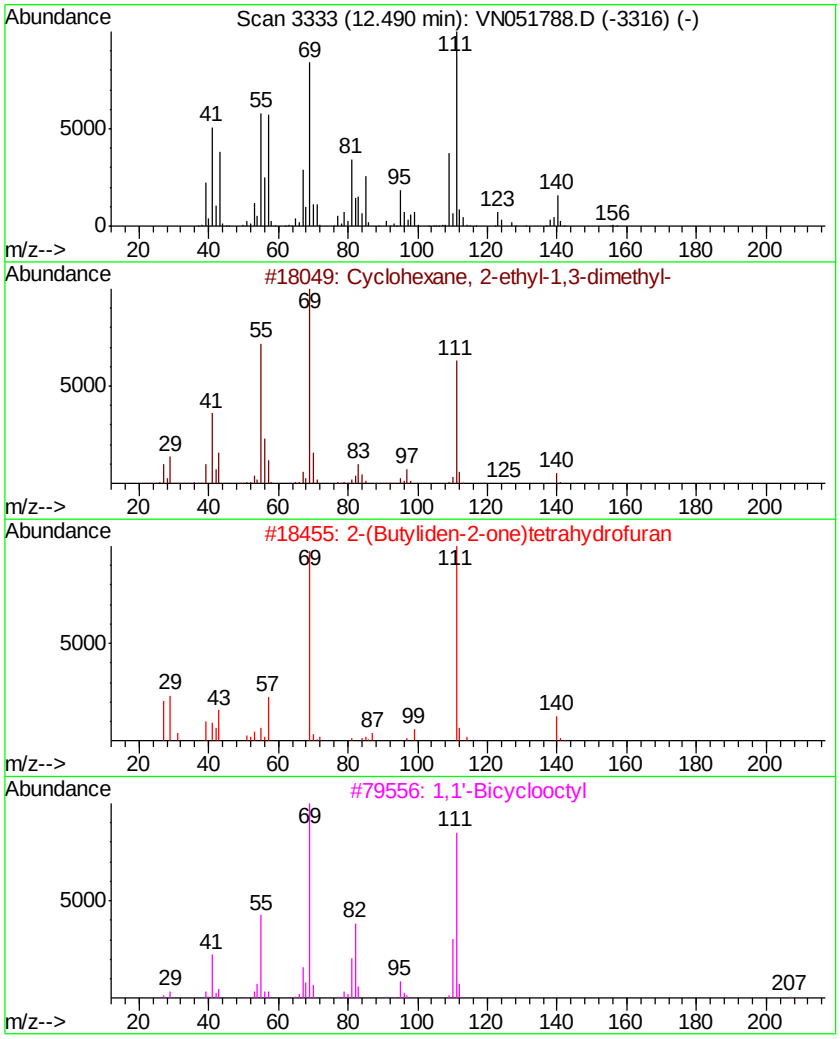
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

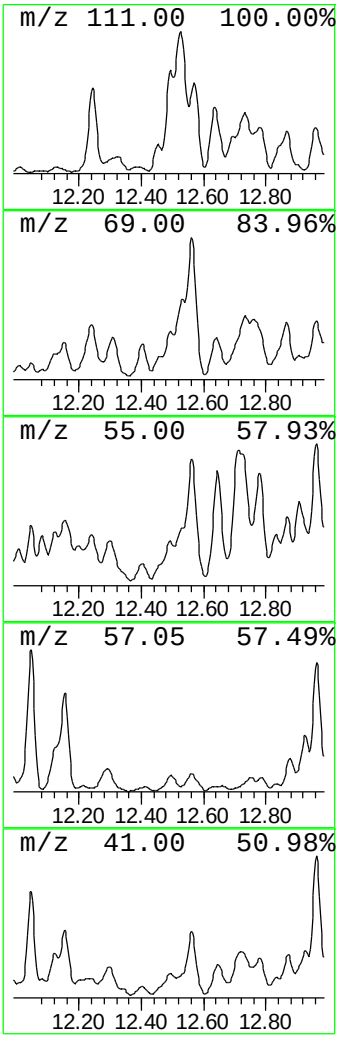
****

Peak Number 5 unknown12.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	99.98 ug/l	4654100	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-ethyl-1,3-dimethyl-	140	C10H20	007045-67-2	49
2	2-(Butyliden-2-one)tetrahydrofuran	140	C8H12O2	343270-50-8	49
3	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	47
4	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	47
5	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	47





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Instrument : MSVOA_N
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

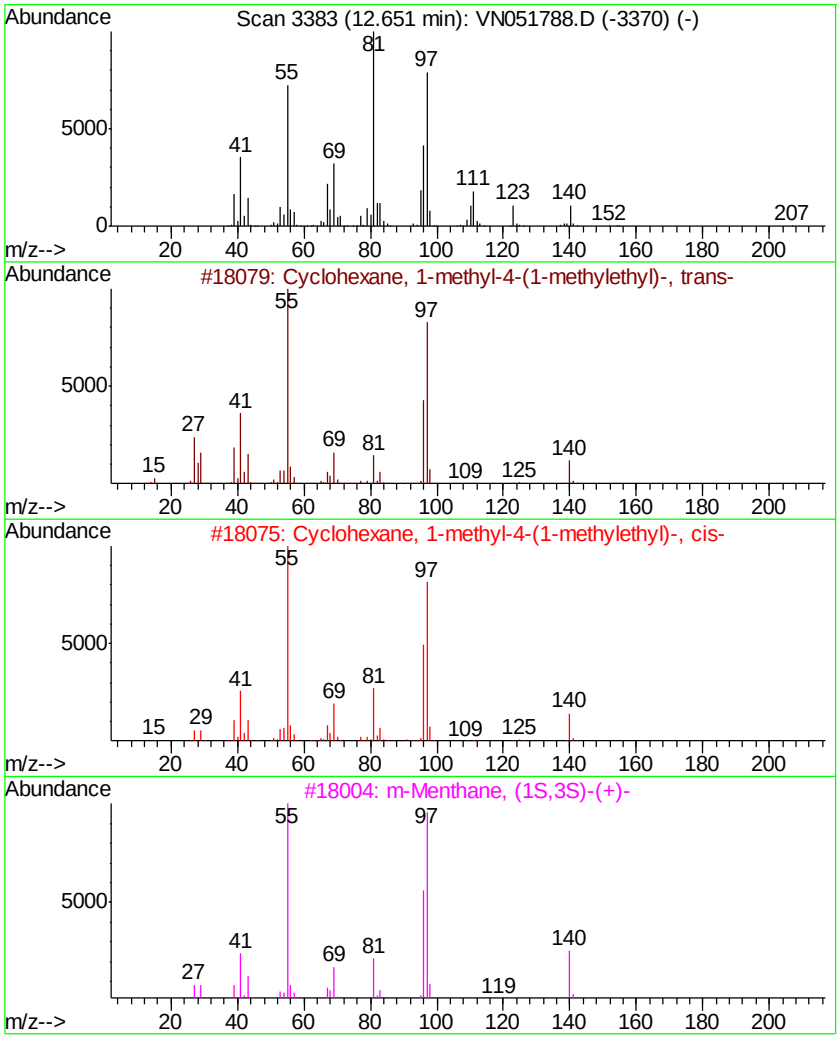
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

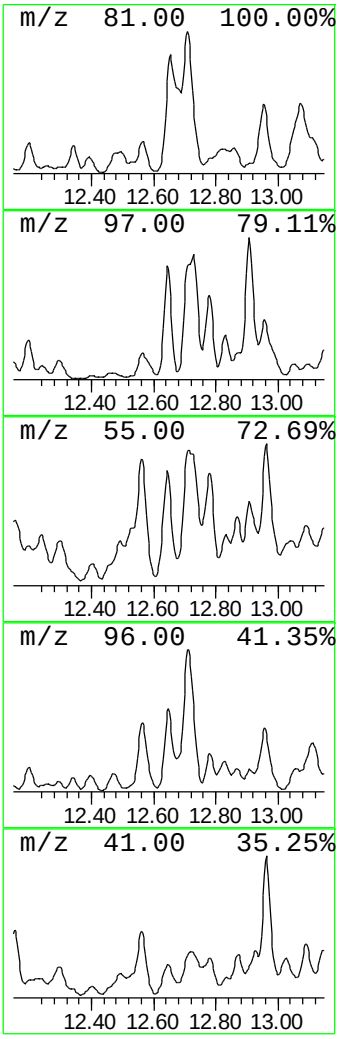
****

Peak Number 6 unknown12.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	137.36 ug/l	6394270	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	49
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49
3	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	47
4	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	47
5	Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	43





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ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

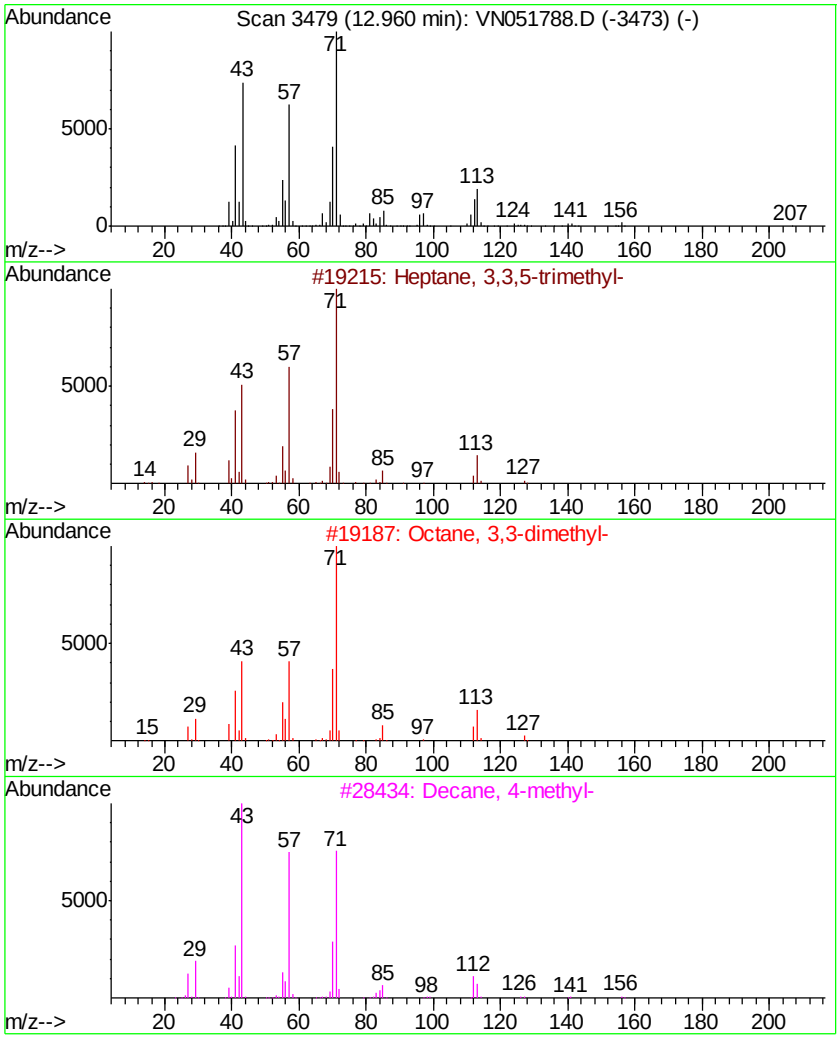
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

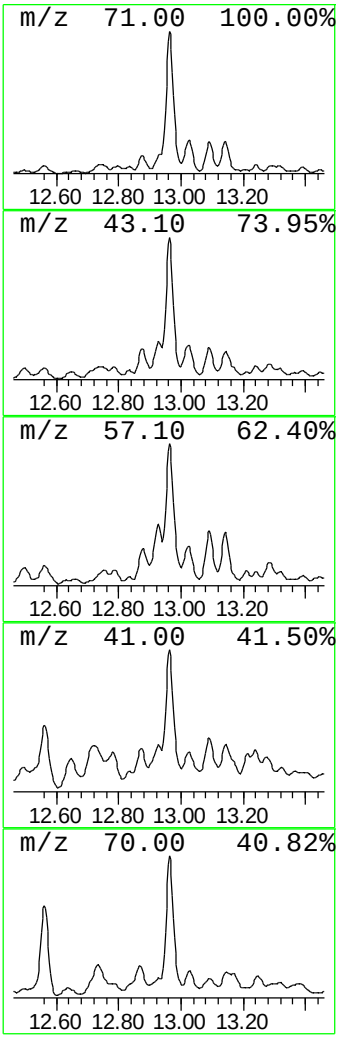
****

Peak Number 8 Heptane, 3,3,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	285.08 ug/l	13270400	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	80
2	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78
3	Decane, 4-methyl-	156	C11H24	002847-72-5	74
4	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

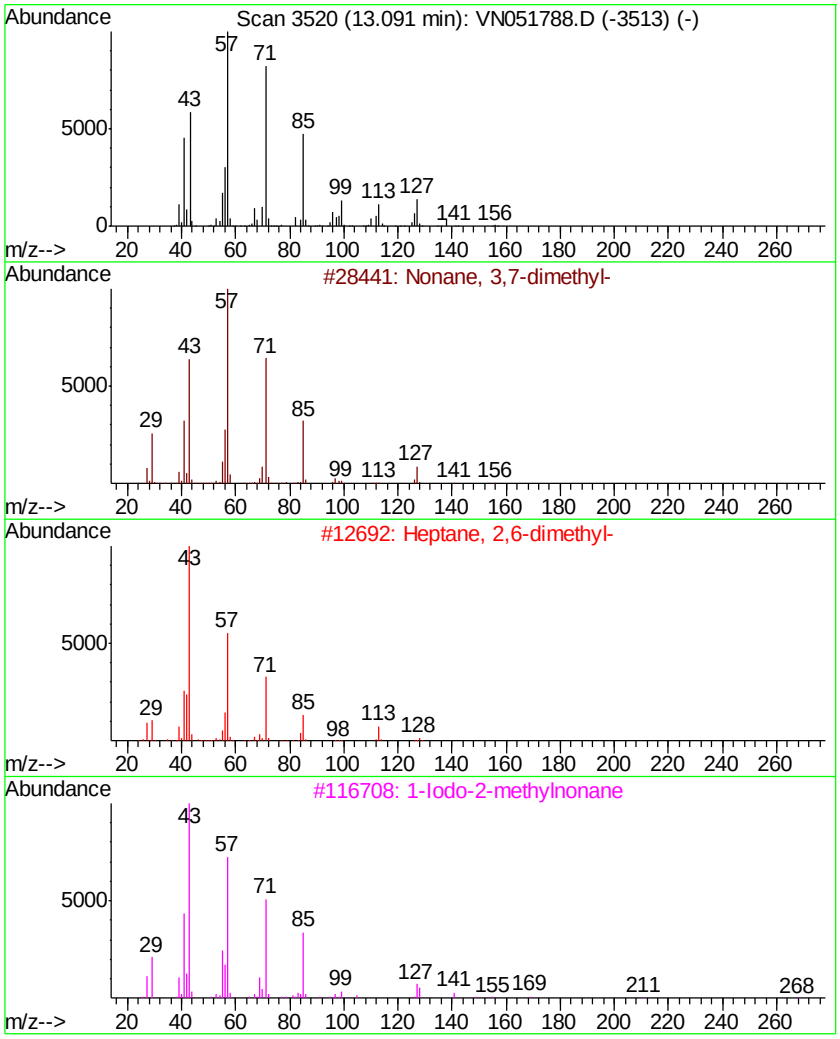
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

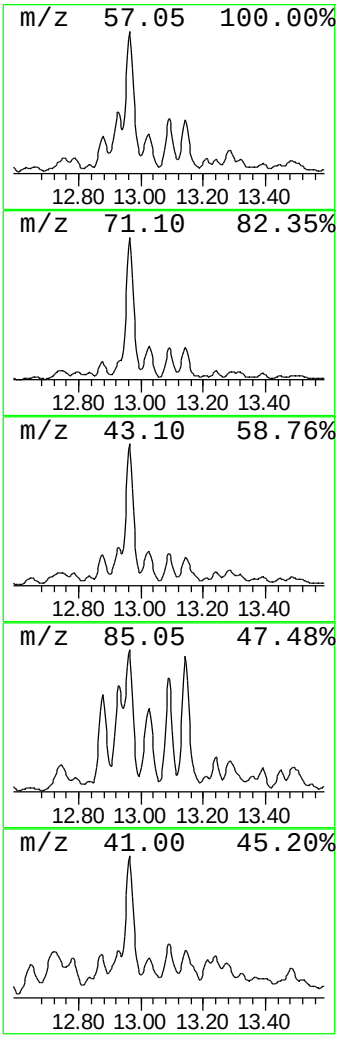
****

Peak Number 9 Nonane, 3,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	59.22 ug/l	2756570	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
2	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	87
3	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	72
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
5	Decane, 3-methyl-	156	C11H24	013151-34-3	68





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

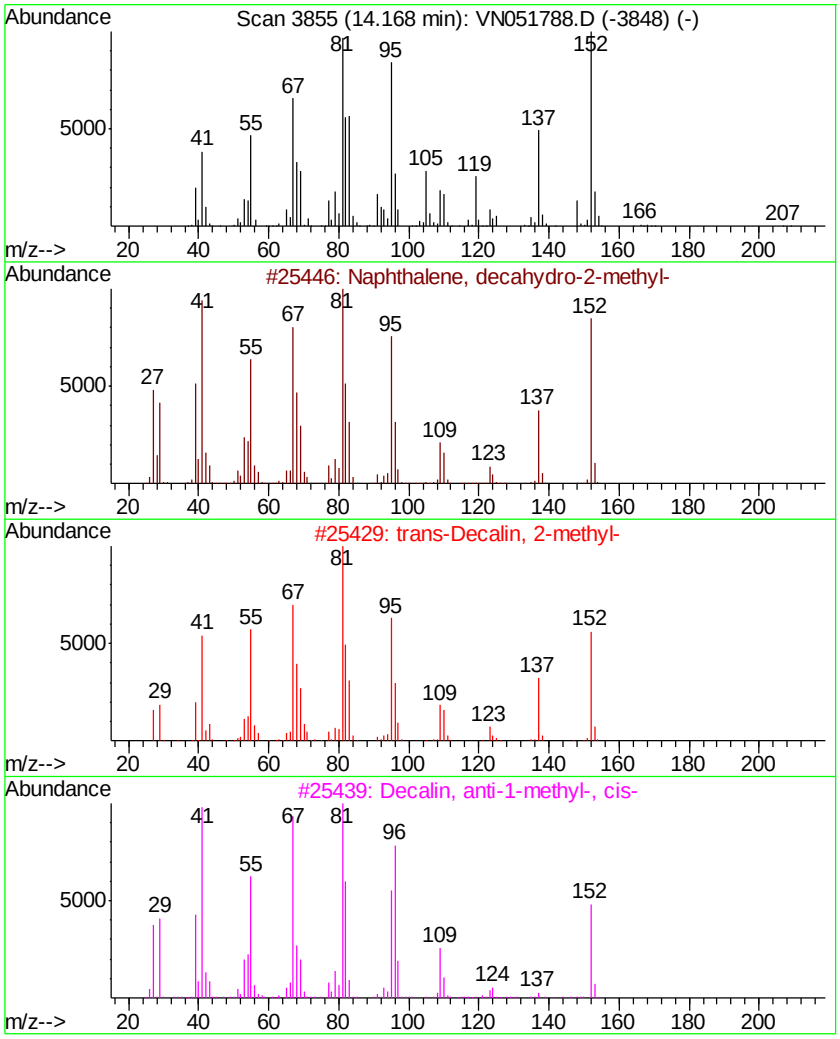
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

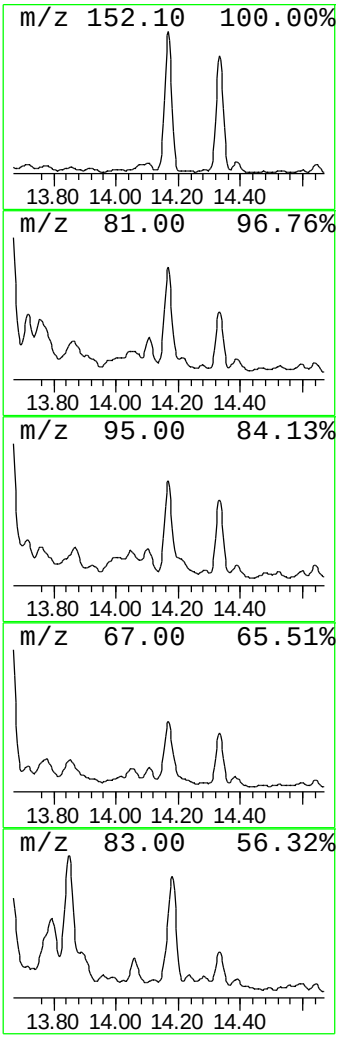
****

Peak Number 10 Naphthalene, decahydro-2-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	78.61 ug/l	3659400	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	86
3	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	60
4	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	58
5	trans,trans-3-Ethylbicyclo[4.4.0...	166	C12H22	058462-32-1	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051788.D
Acq On : 10 Oct 2018 14:05
Operator : MD\SY
Sample : J5165-19 10X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-B(8-12)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.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
unknown11.92	11.92	110.0	ug/l	7371530	3	11.41	3351230	50.0
Octane, 2,6-dimet...	12.05	96.3	ug/l	6457770	3	11.41	3351230	50.0
Octane, 3,5-dimet...	12.12	50.9	ug/l	3414430	3	11.41	3351230	50.0
unknown12.15	12.15	63.5	ug/l	4258470	3	11.41	3351230	50.0
unknown12.49	12.49	100.0	ug/l	4654100	4	13.35	2327530	50.0
unknown12.65	12.65	137.4	ug/l	6394270	4	13.35	2327530	50.0
Heptane, 3,3,5-tr...	12.96	285.1	ug/l	13270400	4	13.35	2327530	50.0
Nonane, 3,7-dimet...	13.09	59.2	ug/l	2756570	4	13.35	2327530	50.0
Naphthalene, deca...	14.17	78.6	ug/l	3659400	4	13.35	2327530	50.0