LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

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\82N121818W.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	7.590	1789	1809	1820	rBV	673950	1667794	3.43%	0.315%
2	7.667	1820	1833	1853	rVB	1477798	3503957	7.21%	0.663%
3	8.027	1925	1945	1968	rBV	759665	1768978	3.64%	0.334%
4	8.587	2102	2119	2142	rBV	2120686	4406354	9.07%	0.833%
5	10.091	2572	2587	2612	rVB	3909873	7583250	15.61%	1.434%
6	10.259	2631	2639	2660	rVB6	235252	639090	1.32%	0.121%
7	10.432	2685	2693	2710	rVB	709023	1327487	2.73%	0.251%
8	10.532	2710	2724	2733	rBV2	409285	917745	1.89%	0.174%
9	10.625	2745	2753	2763	rVB	562221	900190	1.85%	0.170%
10	10.718	2771	2782	2794	rVB	2478192	4119899	8.48%	0.779%
11	10.821	2794	2814	2827	rBV	1387801	3086745	6.35%	0.584%
12	10.889	2827	2835	2841	rBV3	552338	912915	1.88%	0.173%
13	10.953	2848	2855	2861	rVB	684439	913394	1.88%	0.173%
14	11.005	2861	2871	2882	rBV2	5120313	8985050	18.50%	1.699%
15	11.059	2883	2888	2895	rVB	620356	821363	1.69%	0.155%
16	11.124	2895	2908	2916	rBV5	3036821	5777333	11.89%	1.092%
17	11.165	2916	2921	2926	rVV2	784576	1149462	2.37%	0.217%
18	11.210	2927	2935	2951	rVB2	3296584	6550598	13.49%	1.239%
19	11.291	2951	2960	2968	rBV	1017143	1700419	3.50%	0.322%
20	11.339	2968	2975	2985	rBV7	316190	551151	1.13%	0.104%
21	11.407	2985	2996	3005	rBV	3034477	5303836	10.92%	1.003%
22	11.493	3016	3023	3030	rBV3	462516	753723	1.55%	0.143%
23	11.542	3030	3038	3045	rVV	1945651	3097301	6.38%	0.586%
24	11.593	3045	3054	3063	rVV6	3433323	7478951	15.40%	1.414%
25	11.654	3064	3073	3081	rVV2	7924165	14965001	30.81%	2.830%
26	11.699	3082	3087	3097	rVB2	5727909	8700070	17.91%	1.645%
27	11.760	3097	3106	3113	rBV3	1421201	2681743	5.52%	0.507%
28	11.853	3128	3135	3143	rVB4	2333959	3390166	6.98%	0.641%
29	11.924	3143	3157	3169	rBV5	10038062	24466189	50.37%	4.626%
30	12.046	3187	3195	3203	rBV	14087693	19207012	39.54%	3.632%
31	12.120	3210	3218	3223	rBV3	8573939	13809185	28.43%	2.611%
32	12.165	3224	3232	3249	rVB4	15600080	30871964	63.56%	5.837%
33	12.246	3252	3257	3264	rVV3	3092529	3874061	7.98%	0.732%
34	12.403	3295	3306	3316	rBV5	4847740	9288957	19.12%	1.756%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

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\82N121818W.M
Title : SW846 8260

35	12.490	3317	3333	3339	rBV7	3934625	11085205	22.82%	2.096%
36	12.564	3348	3356	3372	rVB3	15356163	36455692	75.05%	6.893%
37	12.644	3372	3381	3391	rBV5	5833552	11936774	24.57%	2.257%
38	12.728	3393	3407	3416	rVV5	17546906	48573902	100.00%	9.184%
39	12.779	3418	3423	3434	rVB2	10334652	16008707	32.96%	3.027%
40	12.869	3444	3451	3458	rBV3	5005465	6918589	14.24%	1.308%
41	12.911	3459	3464	3465	rBV3	2045483	1805669	3.72%	0.341%
42	12.963	3473	3480	3495	rVB3	18012797	31191297	64.21%	5.898%
43	13.169	3532	3544	3552	rVV6	7313440	16624639	34.23%	3.143%
44	13.242	3553	3567	3587	rVB2	14594556	34423746	70.87%	6.509%
45	13.513	3647	3651	3669	rVB2	6286127	12567779	25.87%	2.376%
46	13.612	3670	3682	3689	rBV2	5722086	11908361	24.52%	2.252%
47	13.664	3689	3698	3708	rVV4	12544579	23897739	49.20%	4.518%
48	13.712	3709	3713	3721	rVB2	2290518	2912768	6.00%	0.551%
49	13.889	3761	3768	3778	rVB	11333578	17480770	35.99%	3.305%
50	13.995	3792	3801	3811	rVB4	6080820	11216407	23.09%	2.121%
51	14.178	3849	3858	3864	rBV5	3869275	7595243	15.64%	1.436%
52	14.291	3885	3893	3899	rBV	1869062	2880031	5.93%	0.545%
53	14.332	3900	3906	3912	rVV2	1761944	2422246	4.99%	0.458%
54	14.484	3946	3953	3960	rBV3	429894	798350	1.64%	0.151%
55	14.525	3961	3966	3974	rVB3	758392	1049204	2.16%	0.198%
56	14.583	3974	3984	3997	rBV4	4138447	8221277	16.93%	1.554%
57	14.648	3997	4004	4015	rVB2	1301651	2186188	4.50%	0.413%
58	14.850	4061	4067	4073	rVB3	611092	786538	1.62%	0.149%
59	14.885	4074	4078	4090	rVV2	558458	933106	1.92%	0.176%
60	14.956	4092	4100	4111	rVB4	918573	1836093	3.78%	0.347%

Sum of corrected areas: 528887653

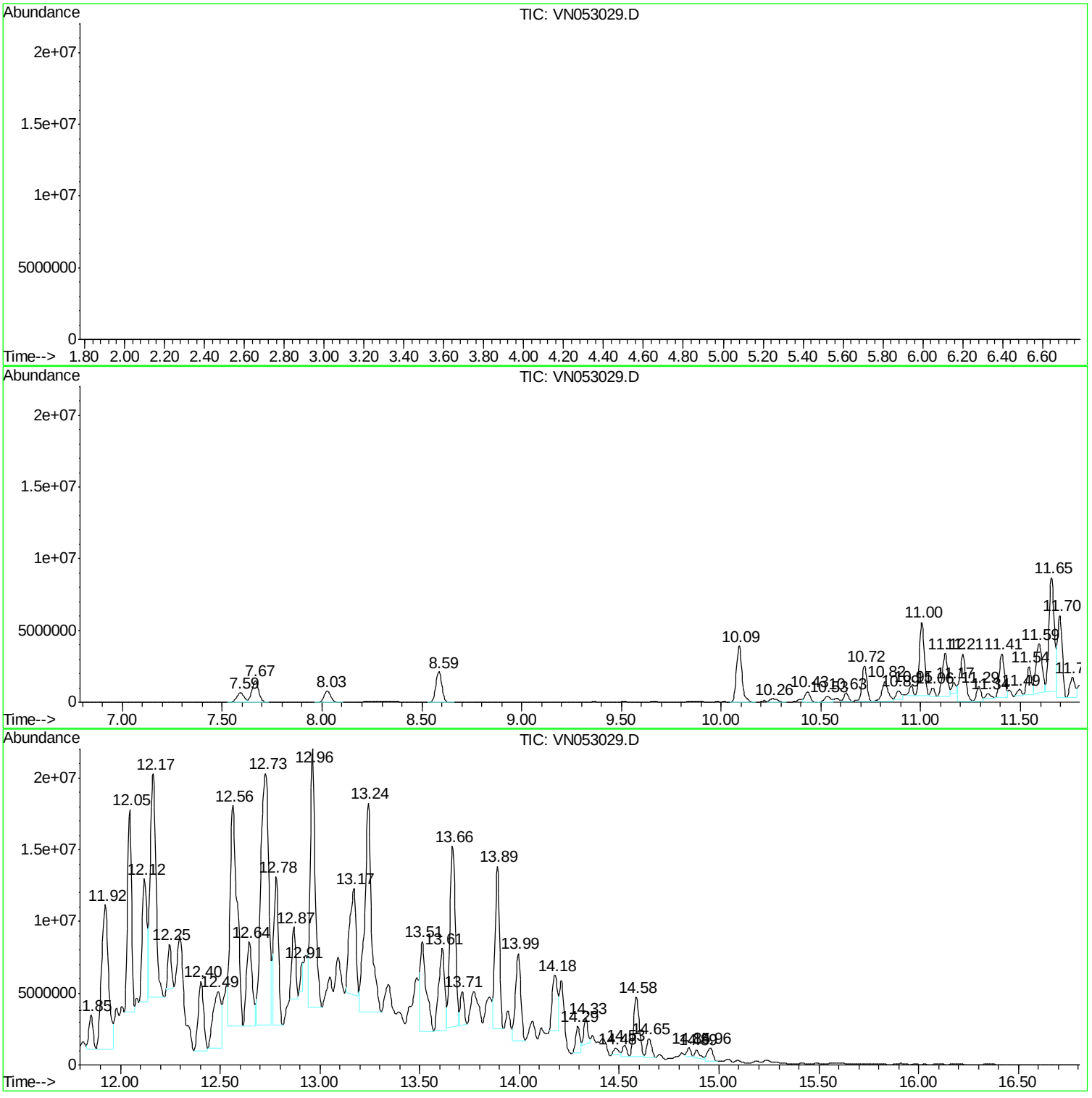
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

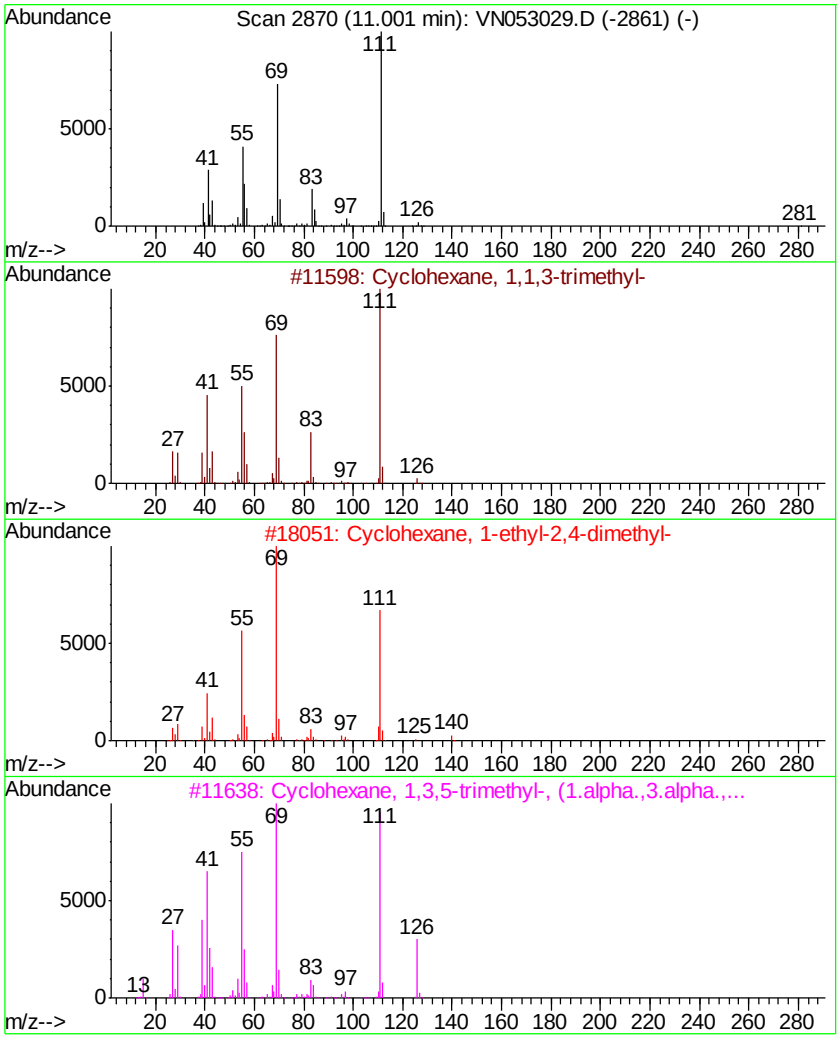
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

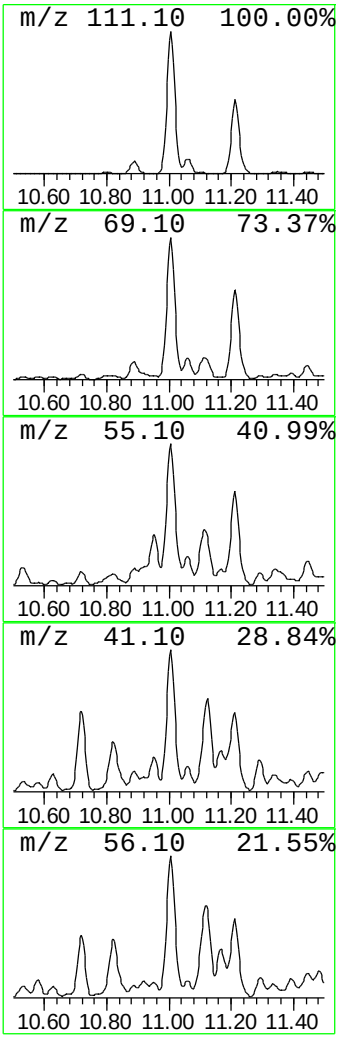
****

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	84.70 ug/l	8985050	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	72
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	64
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	59
5	4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	58





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

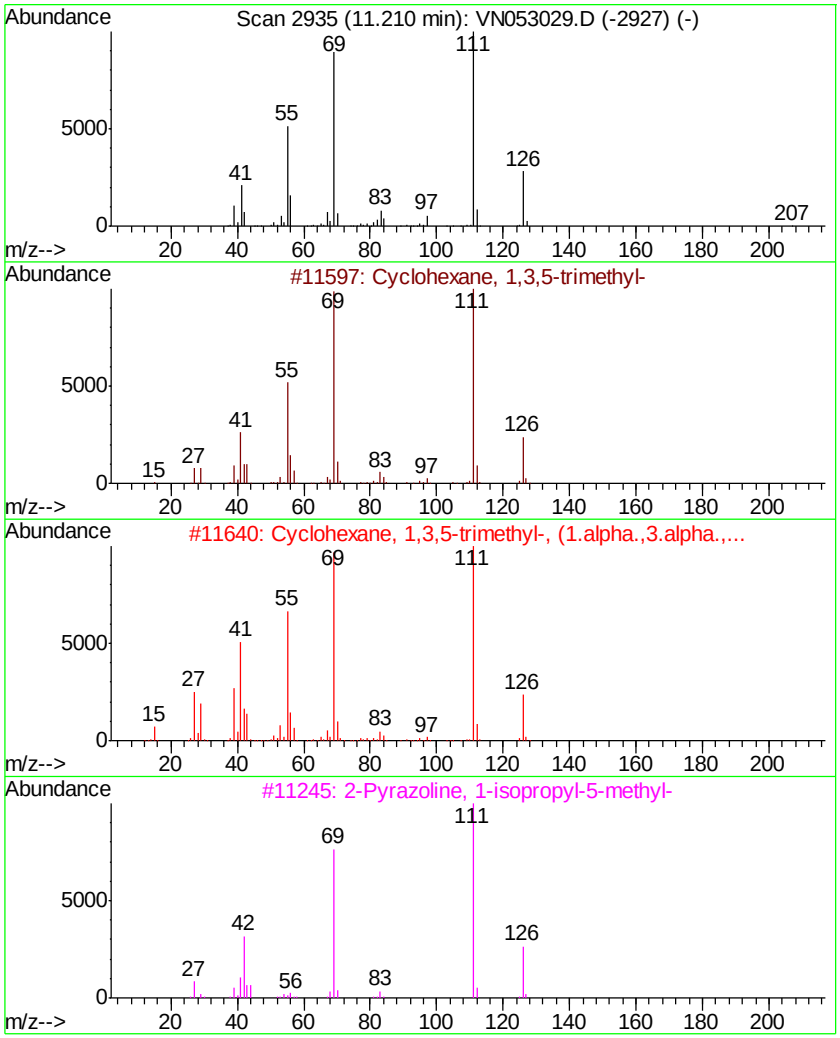
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

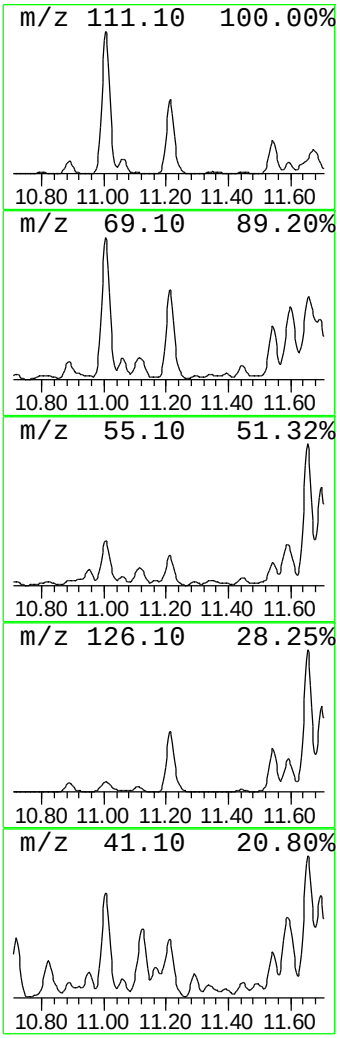
****

Peak Number 2 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	61.75 ug/l	6550600	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	91
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	86
3	2-Pyrazoline, 1-isopropyl-5-methyl-	126	C7H14N2	026964-54-5	80
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	74
5	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

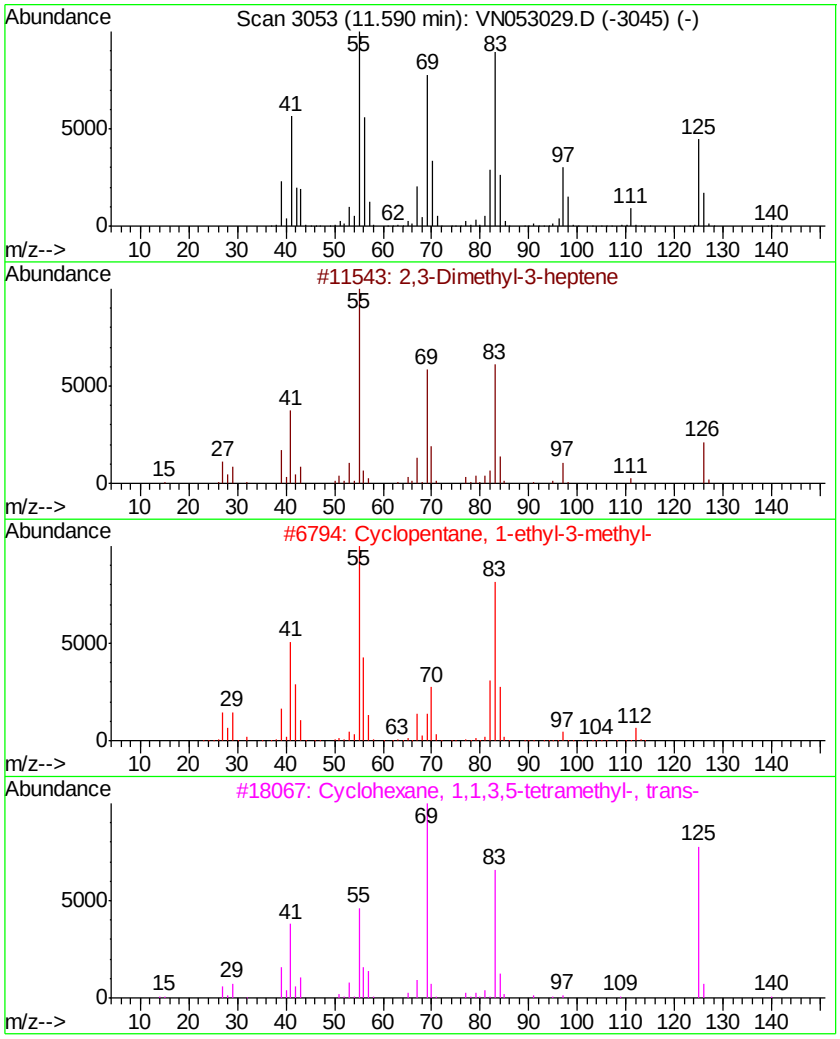
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

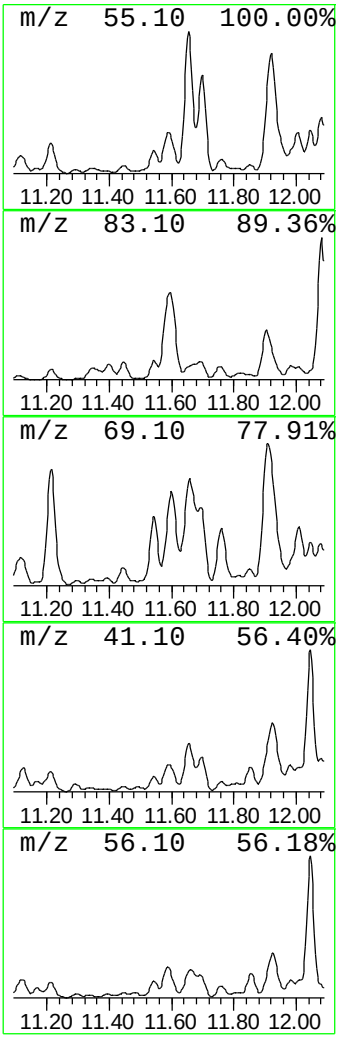
****

Peak Number 3 2,3-Dimethyl-3-heptene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	70.51 ug/l	7478950	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	64
2	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	50
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	46
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
5	3-Undecene, 5-methyl-	168	C12H24	1000061-84-1	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

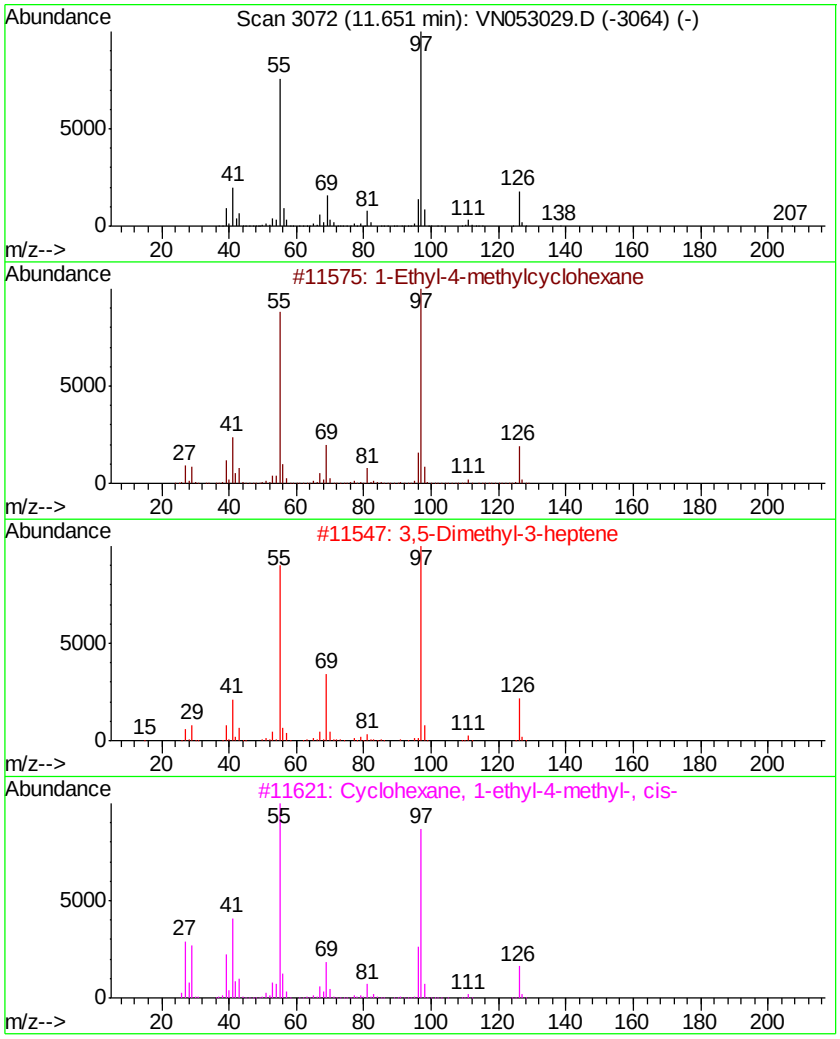
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

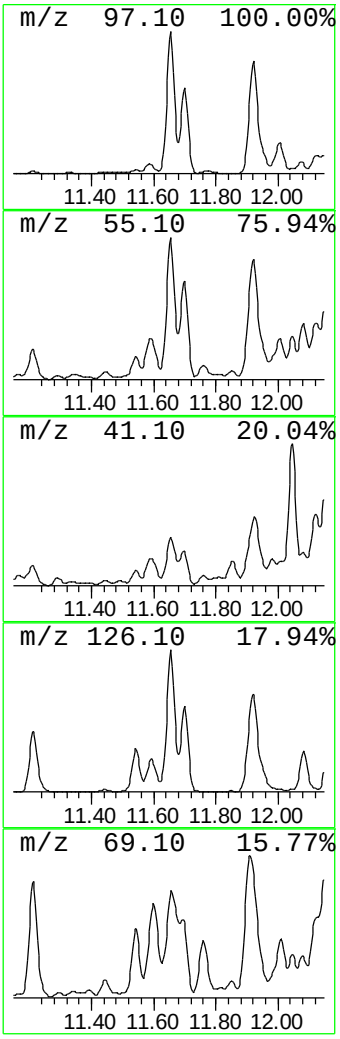
****

Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	141.08 ug/l	14965000	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	86
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	78
5	4-Octen-3-one	126	C8H14O	014129-48-7	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

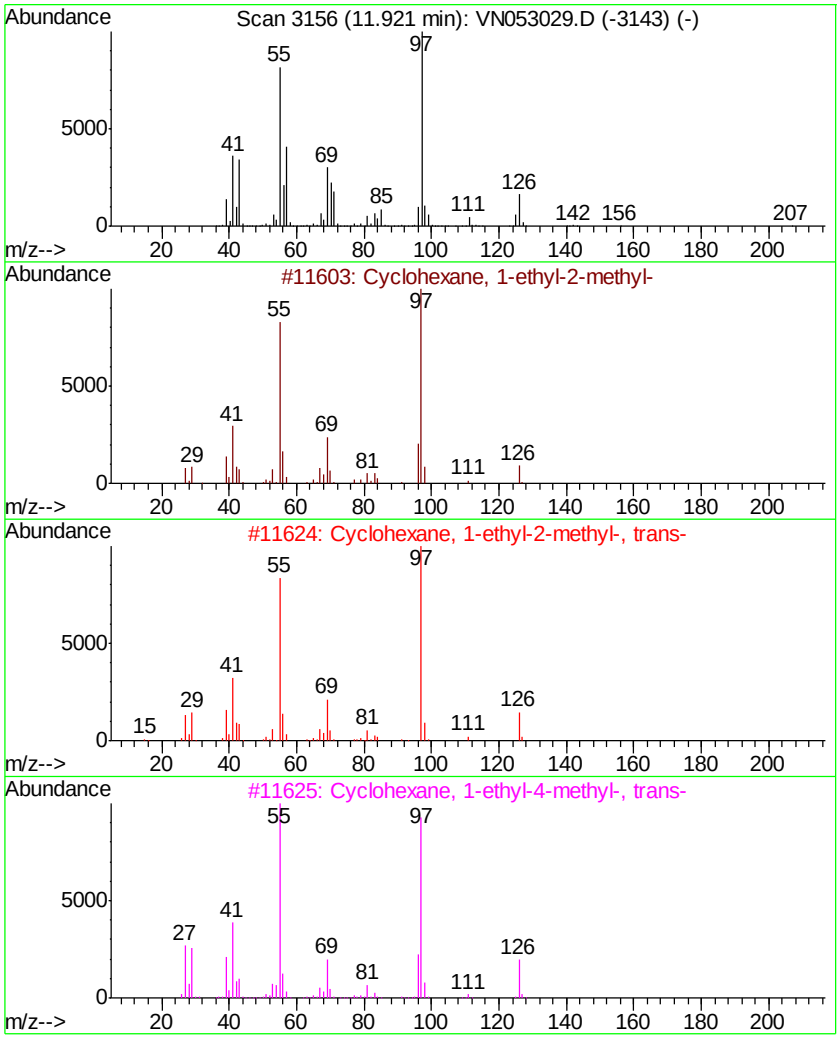
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

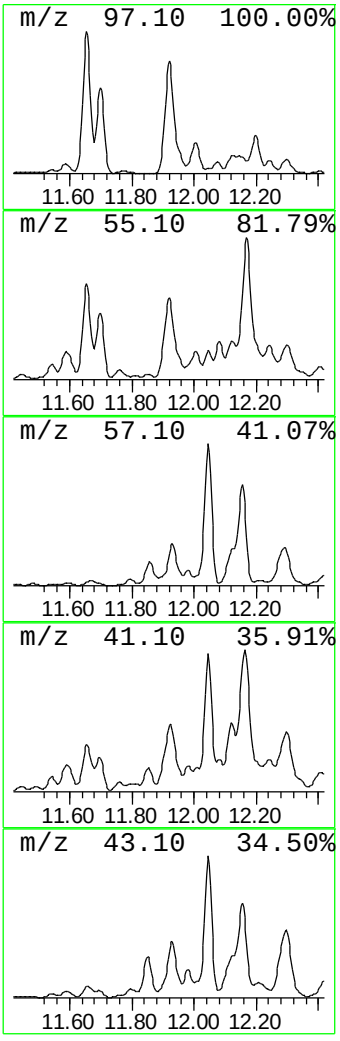
****

Peak Number 6 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	230.65 ug/l	24466200	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	64
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	58
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	58
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
5	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

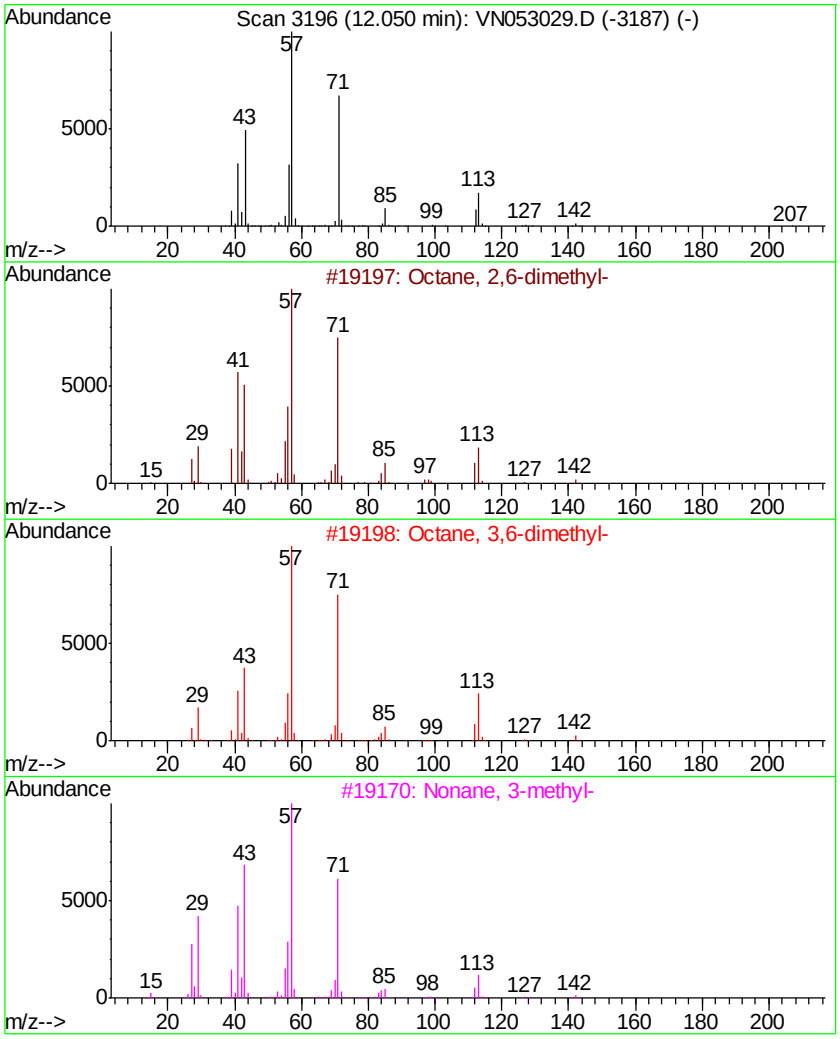
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

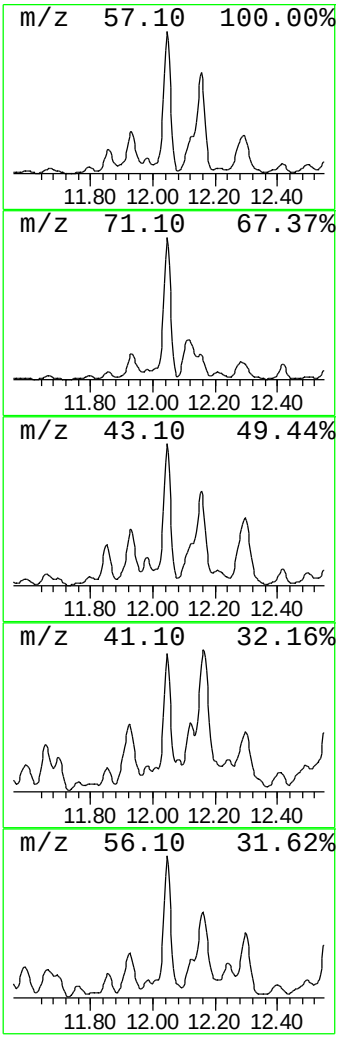
****

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	181.07 ug/l	19207000	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	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	72
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

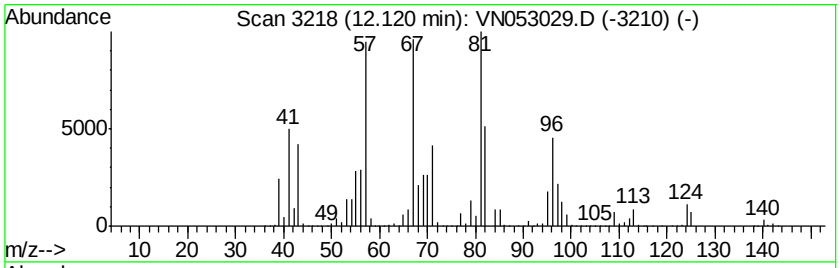
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

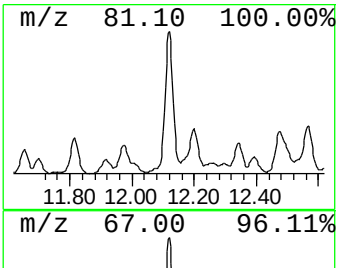
****

Peak Number 8 Pentalene, octahydro-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	130.18 ug/l	13809200	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	78
2	Cyclohexane, methylene-	96	C7H12	001192-37-6	49
3	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
4	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	49
5	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

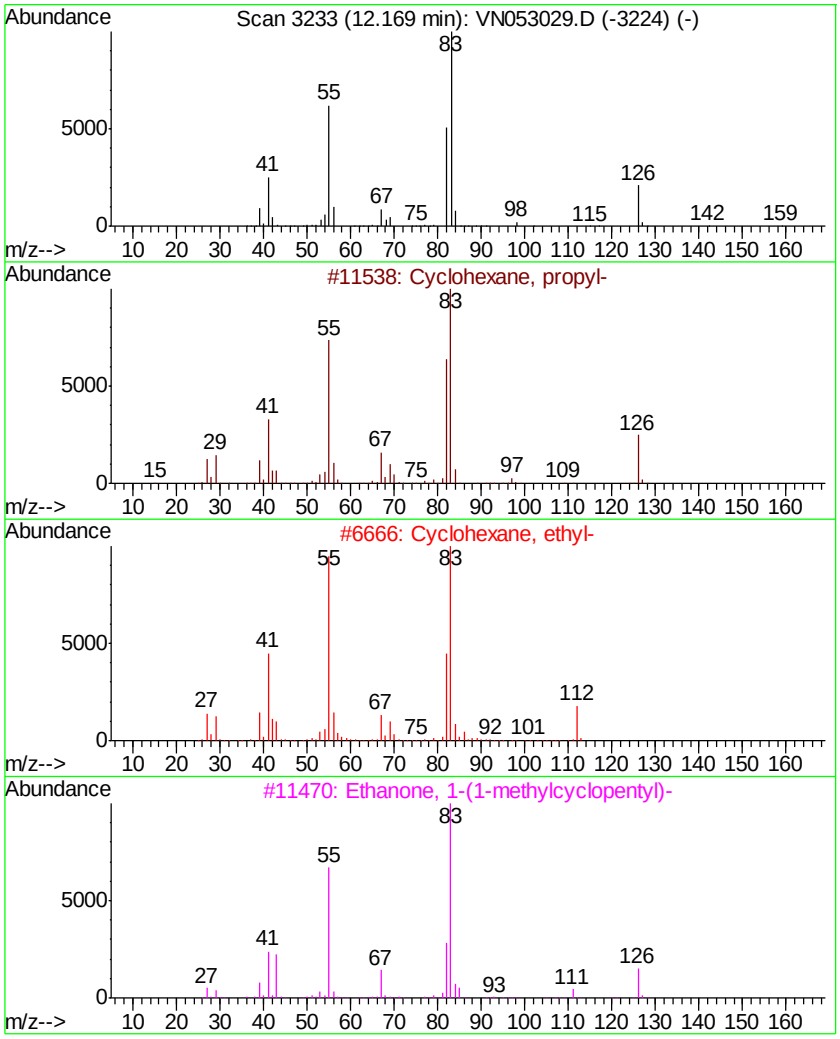
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

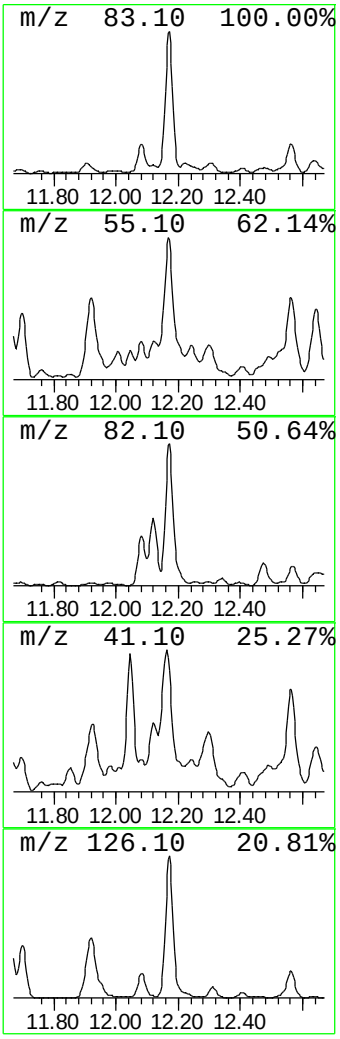
****

Peak Number 9 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	291.03 ug/l	30872000	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
3	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59
4	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	59
5	Oxalic acid, cyclohexyl decyl ester	312	C18H32O4	1000309-31-2	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

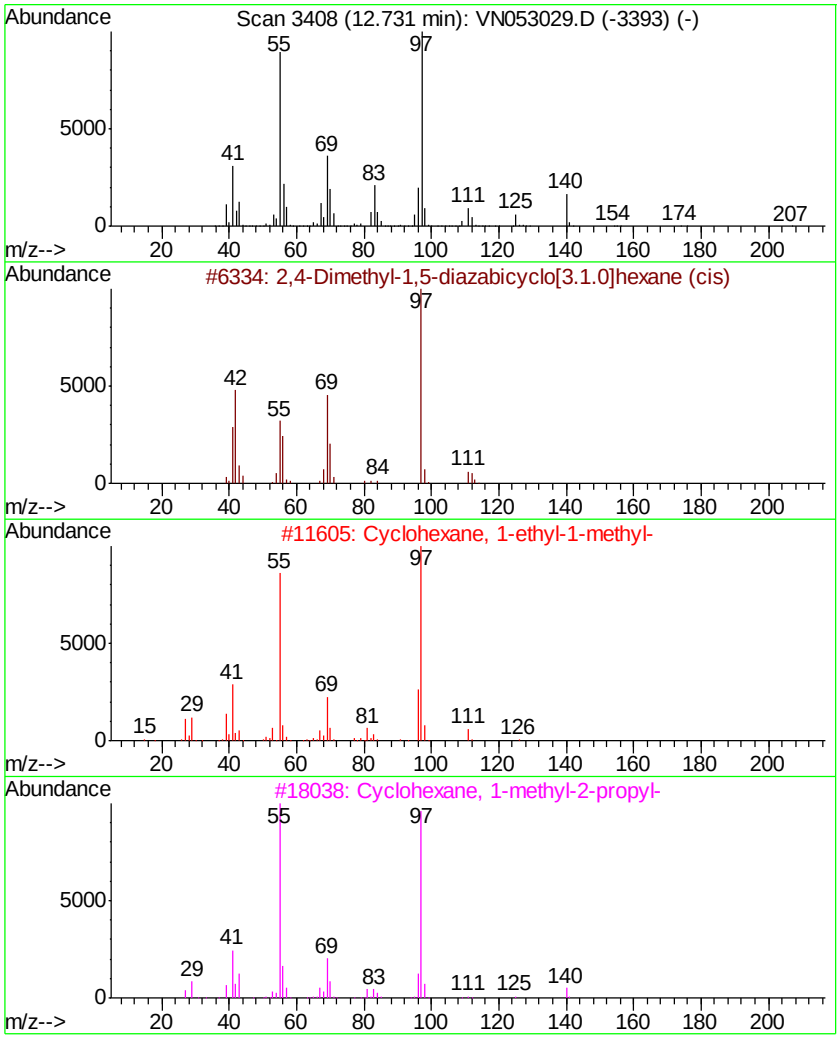
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

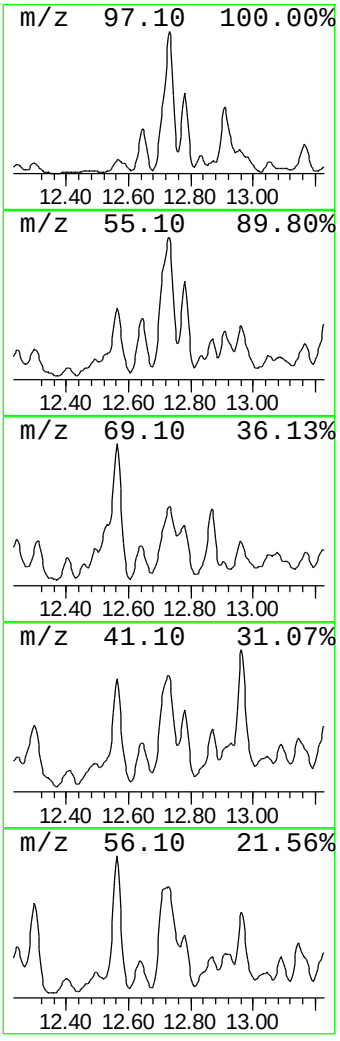
****

Peak Number 10 2,4-Dimethyl-1,5-diazabicyc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	70.55 ug/l	48573900	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	58
2	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	58
3	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	53
4	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	53
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053029.D
Acq On : 20 Dec 2018 00:10
Operator : MD\SY
Sample : J6411-02 10X
Misc : 5.65g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-1B(8-9FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.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
Cyclohexane, 1,1,...	11.00	84.7	ug/l	8985050	3	11.41	5303840	50.0
Cyclohexane, 1,3,...	11.21	61.8	ug/l	6550600	3	11.41	5303840	50.0
2,3-Dimethyl-3-he...	11.59	70.5	ug/l	7478950	3	11.41	5303840	50.0
1-Ethyl-4-methylc...	11.65	141.1	ug/l	14965000	3	11.41	5303840	50.0
Cyclohexane, 1-et...	11.92	230.7	ug/l	24466200	3	11.41	5303840	50.0
Octane, 2,6-dimet...	12.05	181.1	ug/l	19207000	3	11.41	5303840	50.0
Pentalene, octahy...	12.12	130.2	ug/l	13809200	3	11.41	5303840	50.0
Cyclohexane, propyl-	12.17	291.0	ug/l	30872000	3	11.41	5303840	50.0
2,4-Dimethyl-1,5-...	12.73	70.5	ug/l	48573900	4	13.35	34423700	50.0