LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

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\82N032019W.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	2.510	205	229	230	rBV10	41611	103868	2.41%	0.161%
2	4.503	829	849	875	rBV3	42355	156569	3.63%	0.242%
3	5.027	998	1012	1028	rVB5	14438	49680	1.15%	0.077%
4	6.339	1400	1420	1446	rVB2	81765	286493	6.65%	0.443%
5	6.506	1448	1472	1496	rBV2	158191	515705	11.96%	0.798%
6	6.812	1545	1567	1587	rVB6	29189	107674	2.50%	0.167%
7	7.378	1719	1743	1765	rVB2	96223	291420	6.76%	0.451%
8	7.590	1788	1809	1819	rBV	369147	911065	21.14%	1.409%
9	7.661	1819	1831	1843	rVV	688602	1675647	38.87%	2.592%
10	7.735	1843	1854	1879	rVB2	482962	1285889	29.83%	1.989%
11	7.928	1899	1914	1929	rVB3	75595	193883	4.50%	0.300%
12	8.024	1929	1944	1965	rBV	425166	989223	22.95%	1.530%
13	8.143	1965	1981	1996	rBV2	117716	292176	6.78%	0.452%
14	8.294	2018	2028	2042	rVB5	49228	110042	2.55%	0.170%
15	8.583	2103	2118	2162	rVB	1029689	2295295	53.25%	3.551%
16	8.895	2201	2215	2230	rVB2	128265	276148	6.41%	0.427%
17	9.043	2242	2261	2267	rBV2	679146	1448047	33.59%	2.240%
18	9.082	2268	2273	2283	rVV	827194	1569253	36.41%	2.427%
19	9.136	2283	2290	2306	rVV	575554	1152241	26.73%	1.782%
20	9.217	2307	2315	2327	rVB3	40425	83100	1.93%	0.129%
21	9.358	2337	2359	2376	rBV2	756984	2165261	50.23%	3.349%
22	9.513	2395	2407	2419	rVB5	83809	175270	4.07%	0.271%
23	9.657	2430	2452	2460	rBV4	113946	282534	6.55%	0.437%
24	9.706	2460	2467	2477	rVB3	105251	191031	4.43%	0.296%
25	9.841	2495	2509	2521	rBV	540416	1070659	24.84%	1.656%
26	9.902	2521	2528	2539	rVB5	67165	139085	3.23%	0.215%
27	9.979	2540	2552	2554	rBV2	153573	240292	5.57%	0.372%
28	10.088	2573	2586	2613	rBV2	1653974	3658205	84.87%	5.659%
29	10.252	2625	2637	2660	rVB	789236	1686183	39.12%	2.608%
30	10.429	2660	2692	2709	rBV	1967297	4310426	100.00%	6.668%
31	10.529	2709	2723	2734	rBV4	799431	1817711	42.17%	2.812%
32	10.625	2746	2753	2761	rVB3	124823	189148	4.39%	0.293%
33	10.677	2761	2769	2771	rBV3	74012	102435	2.38%	0.158%
34	10.818	2797	2813	2827	rBV	1418255	3119160	72.36%	4.825%

LSC Area Percent Report

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Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

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\82N032019W.M
Title : SW846 8260

35	10.889	2827	2835	2839	rBV2	418510	630989	14.64%	0.976%
36	11.005	2860	2871	2879	rBV4	317164	627690	14.56%	0.971%
37	11.059	2879	2888	2898	rVB	586335	991511	23.00%	1.534%
38	11.165	2913	2921	2926	rBV	262883	402082	9.33%	0.622%
39	11.210	2926	2935	2954	rVB	1586272	3092291	71.74%	4.783%
40	11.329	2955	2972	2981	rBV3	115769	281839	6.54%	0.436%
41	11.406	2984	2996	3011	rBV	1276251	2529930	58.69%	3.914%
42	11.542	3029	3038	3046	rVB2	421304	655281	15.20%	1.014%
43	11.596	3047	3055	3062	rBV3	372158	630285	14.62%	0.975%
44	11.661	3063	3075	3082	rBV5	315940	758025	17.59%	1.173%
45	11.754	3096	3104	3108	rBV6	86274	141350	3.28%	0.219%
46	11.805	3109	3120	3129	rBV5	362454	866983	20.11%	1.341%
47	11.857	3130	3136	3142	rBV2	220417	283055	6.57%	0.438%
48	11.918	3142	3155	3168	rBV7	1520503	3946668	91.56%	6.105%
49	12.117	3199	3217	3225	rBV4	979429	2406057	55.82%	3.722%
50	12.204	3236	3244	3262	rBV8	355435	1119996	25.98%	1.733%
51	12.400	3294	3305	3316	rBV	1137316	2068314	47.98%	3.199%
52	12.644	3371	3381	3394	rBV6	449939	1132724	26.28%	1.752%
53	12.866	3446	3450	3457	rVB4	239495	278471	6.46%	0.431%
54	12.959	3474	3479	3492	rVB3	584954	977092	22.67%	1.511%
55	13.088	3512	3519	3529	rVB	463129	727055	16.87%	1.125%
56	13.149	3532	3538	3550	rVB9	212562	490539	11.38%	0.759%
57	13.210	3551	3557	3563	rBV3	299379	462517	10.73%	0.715%
58	13.342	3589	3598	3613	rVB	1093805	1989761	46.16%	3.078%
59	13.660	3688	3697	3709	rVB4	887268	1546692	35.88%	2.393%
60	14.168	3847	3855	3867	rVB6	695285	1317536	30.57%	2.038%
61	14.332	3899	3906	3914	rVB3	450943	684453	15.88%	1.059%
62	14.641	3995	4002	4014	rVB5	409345	665005	15.43%	1.029%

Sum of corrected areas: 64645009

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
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Acq On : 22 Mar 2019 13:03
Operator : JC/SP
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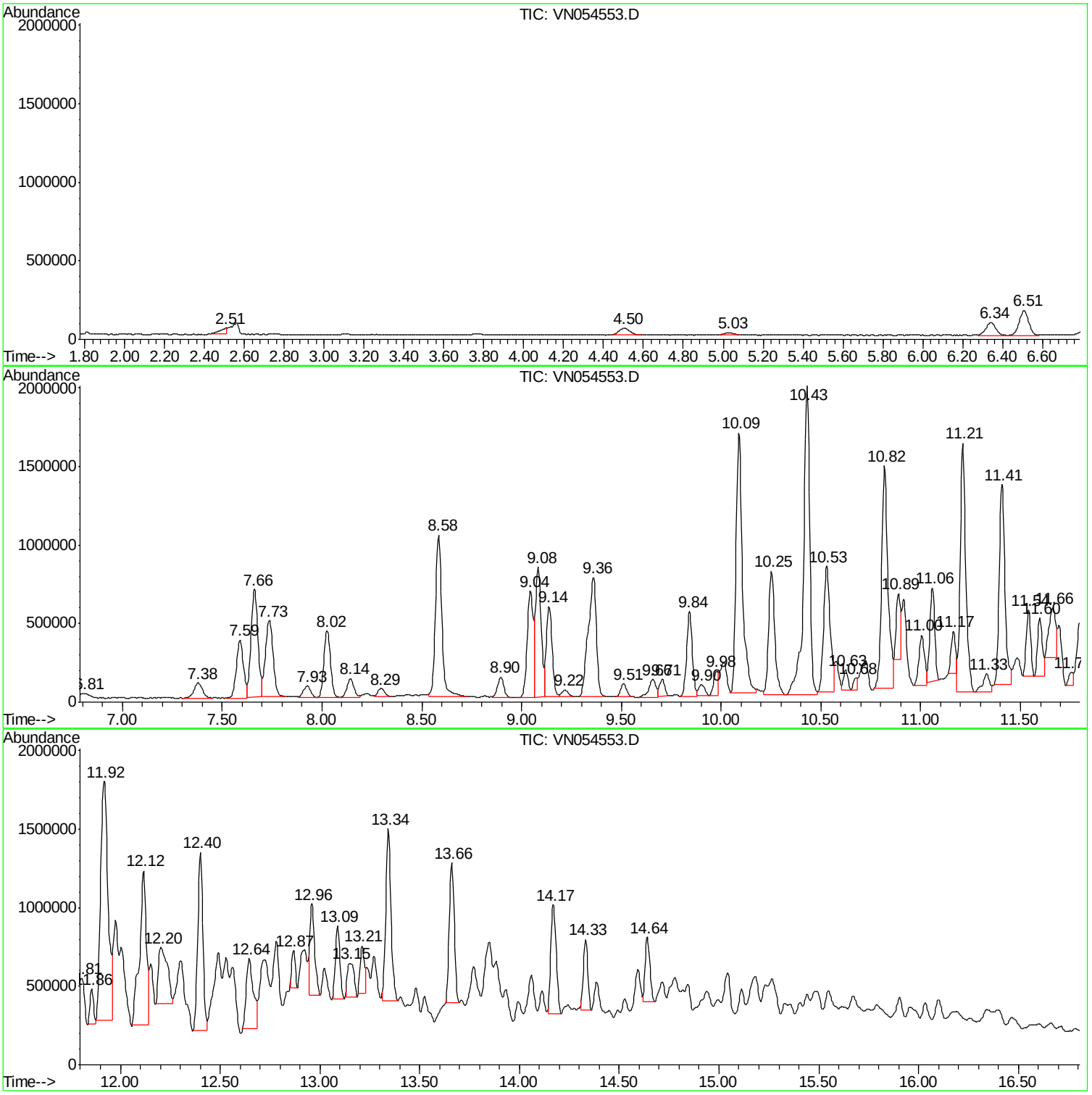
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

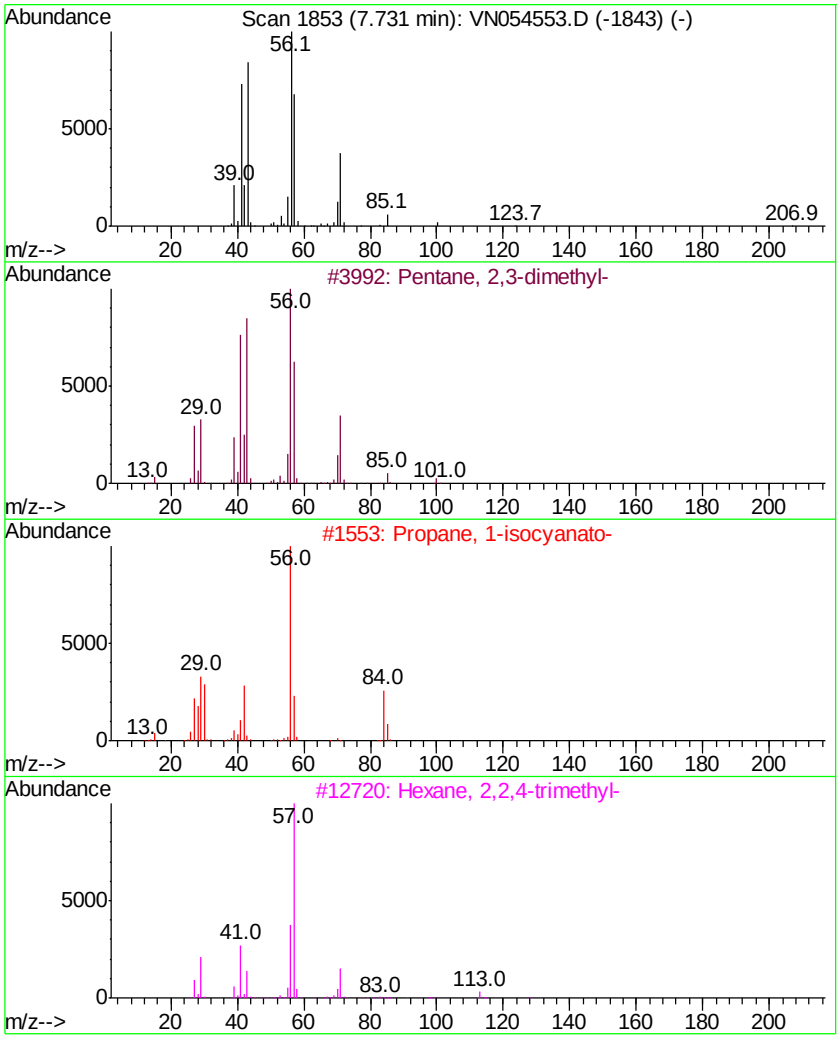
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

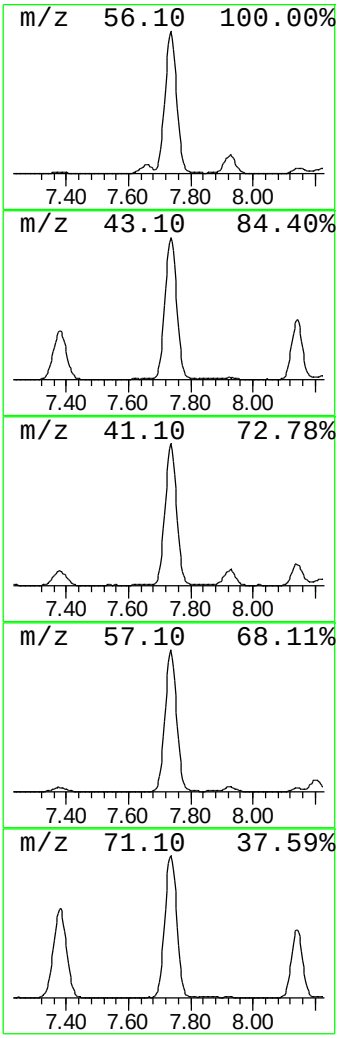
****

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	38.37 ug/l	1285890	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	50
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

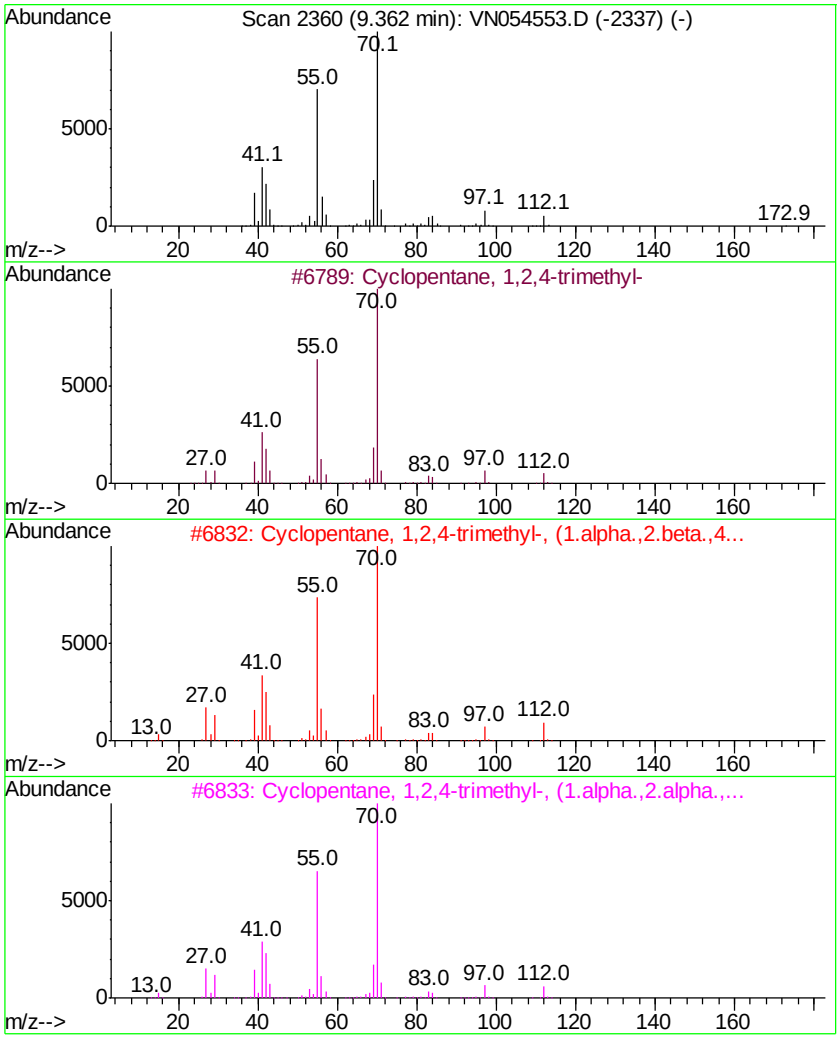
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

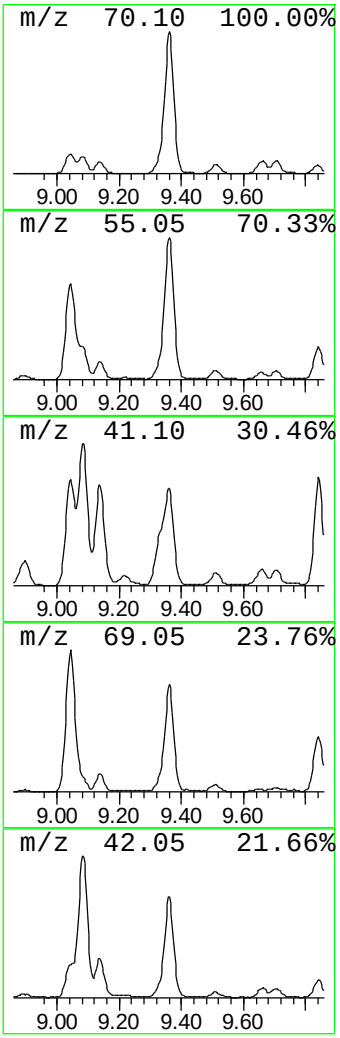
****

Peak Number 2 Cyclopentane, 1,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	47.17 ug/l	2165260	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	94
2	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	91
3	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	90
4	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	80
5	Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
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Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

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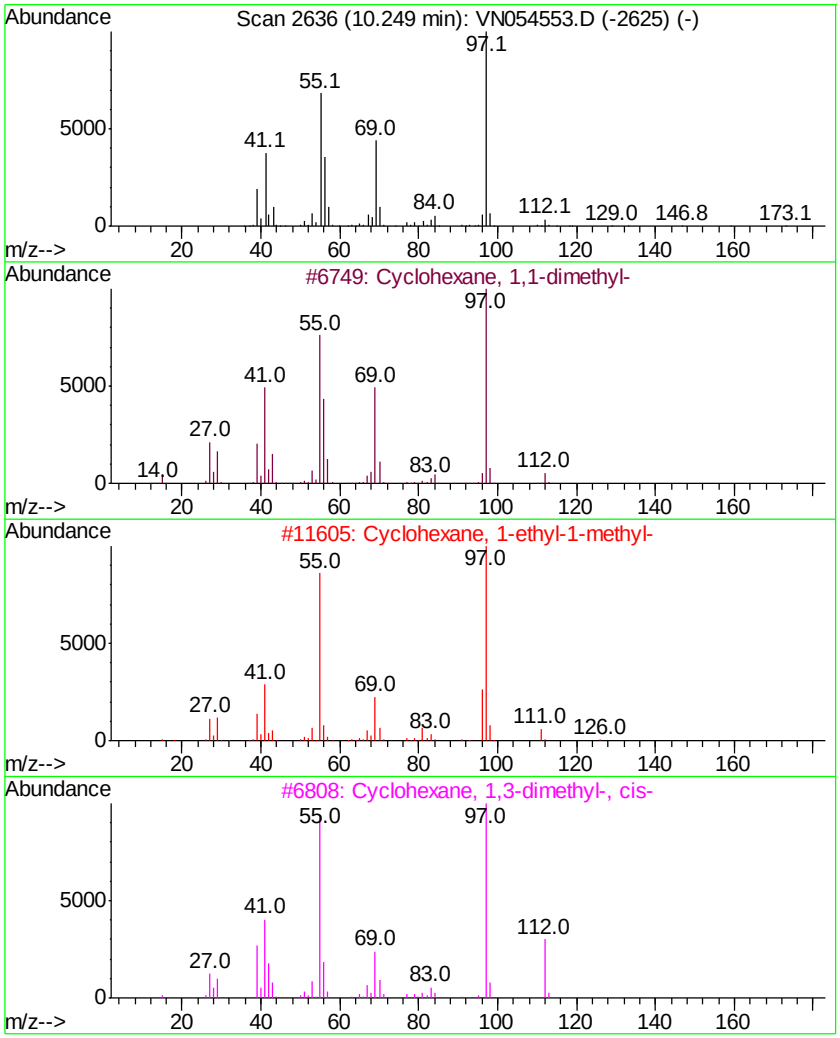
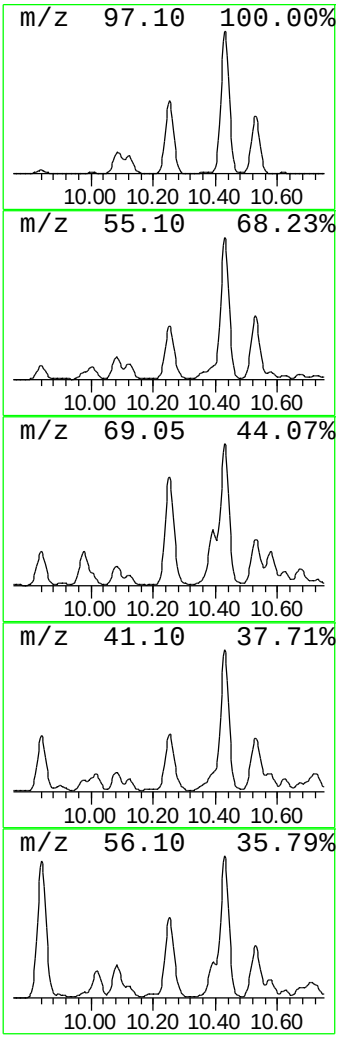
Peak Number 3 Cyclohexane, 1,1-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	33.32 ug/l	1686180	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	97
2	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	59
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
4	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	50
5	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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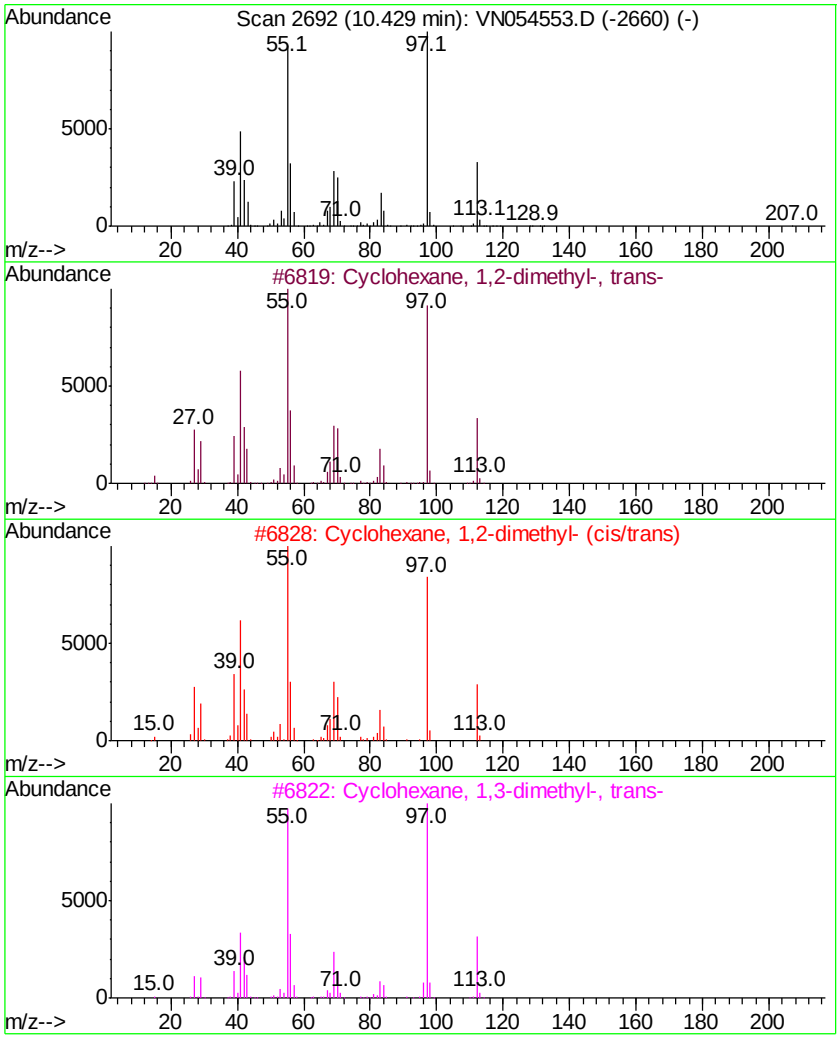
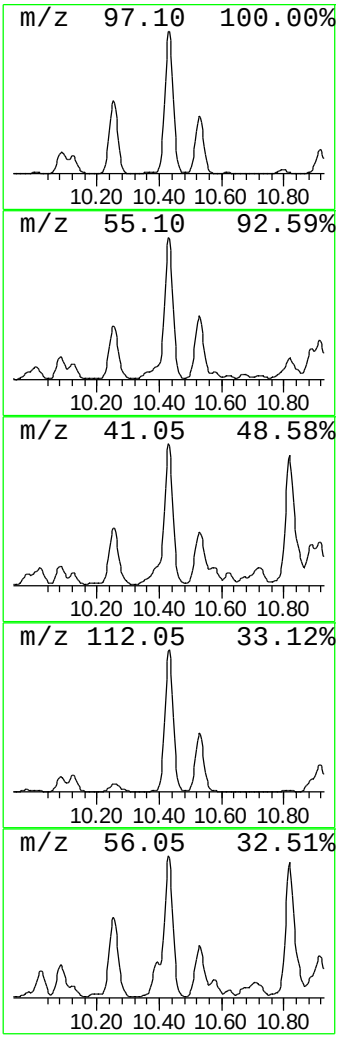
****

Peak Number 4 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	85.19 ug/l	4310430	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	96
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	93
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	90
5	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	83





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Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

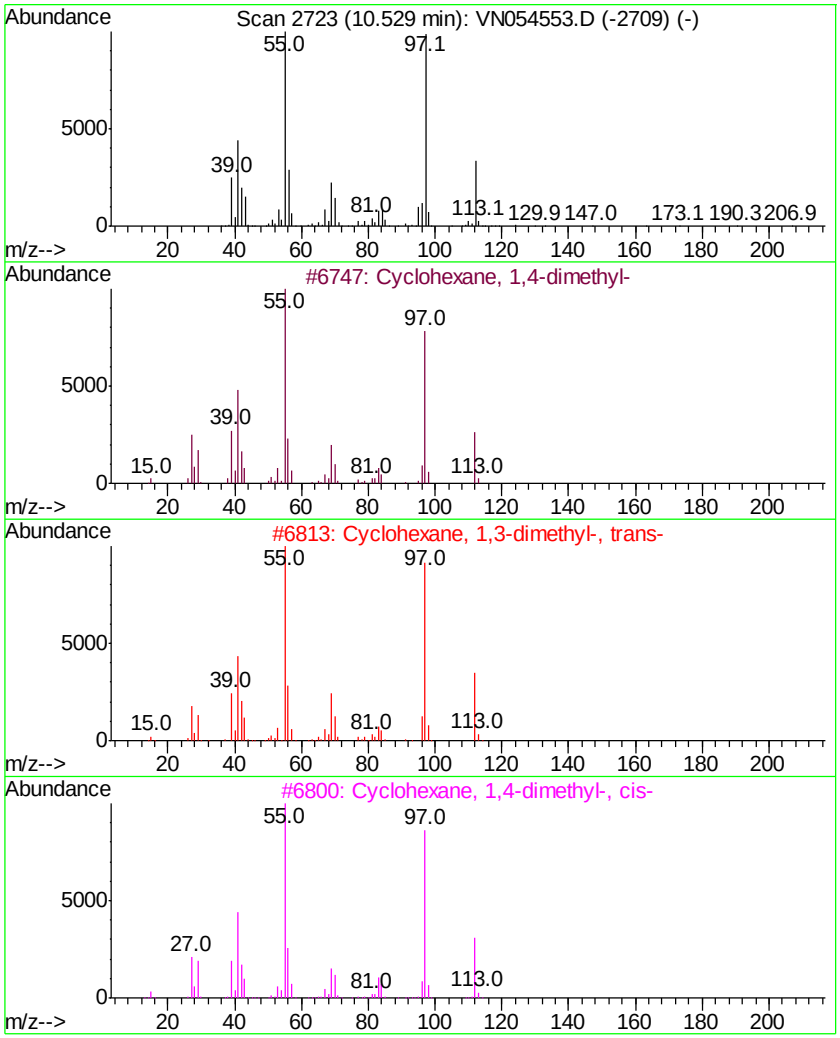
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

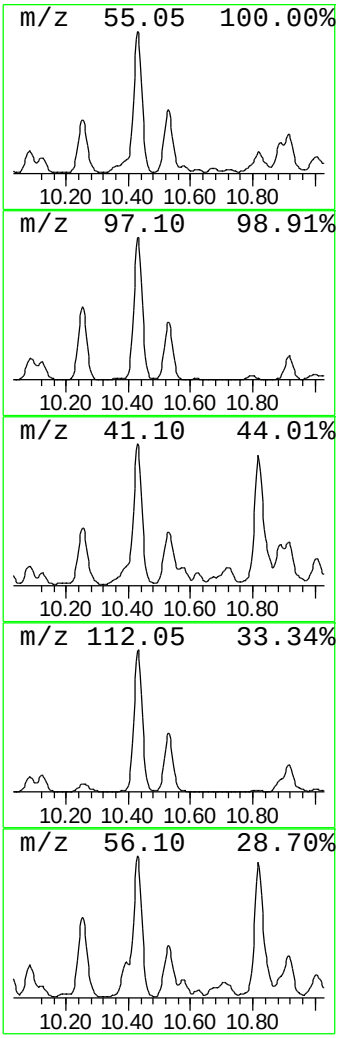
****

Peak Number 5 Cyclohexane, 1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	35.92 ug/l	1817710	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	97
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	96
3	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	94
4	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	90
5	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87





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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

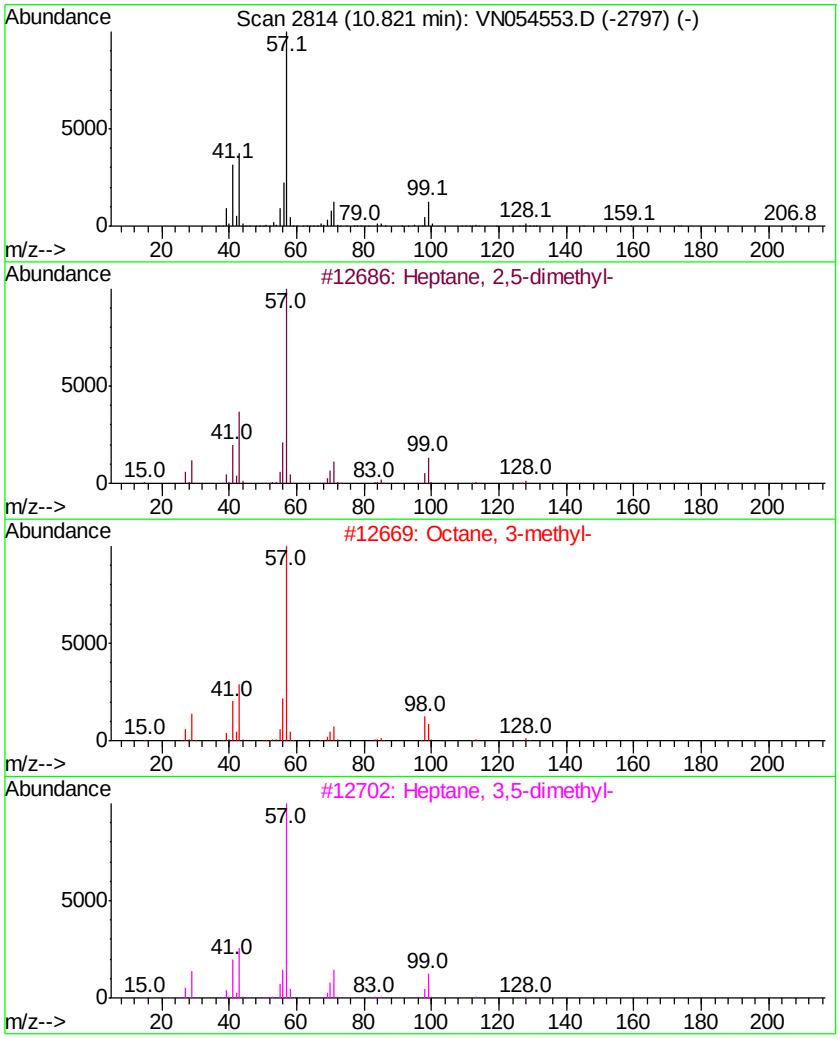
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

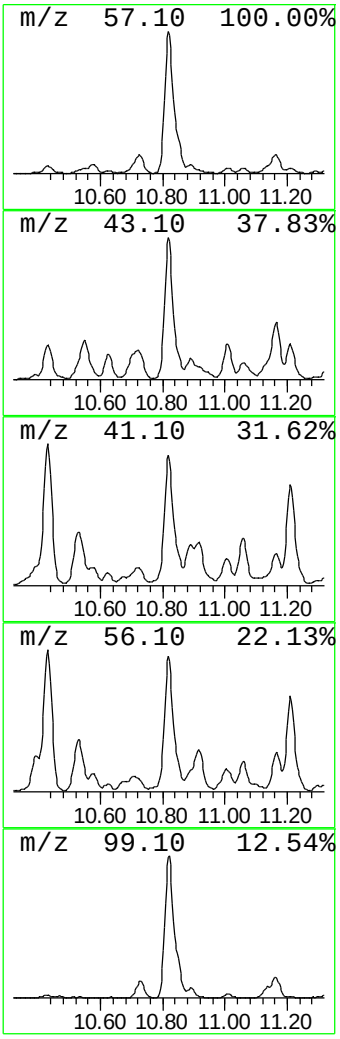
****

Peak Number 6 Heptane, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	61.65 ug/l	3119160	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	91
2	Octane, 3-methyl-	128	C9H20	002216-33-3	90
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	90
4	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	53
5	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
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Sample : K2004-09
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Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

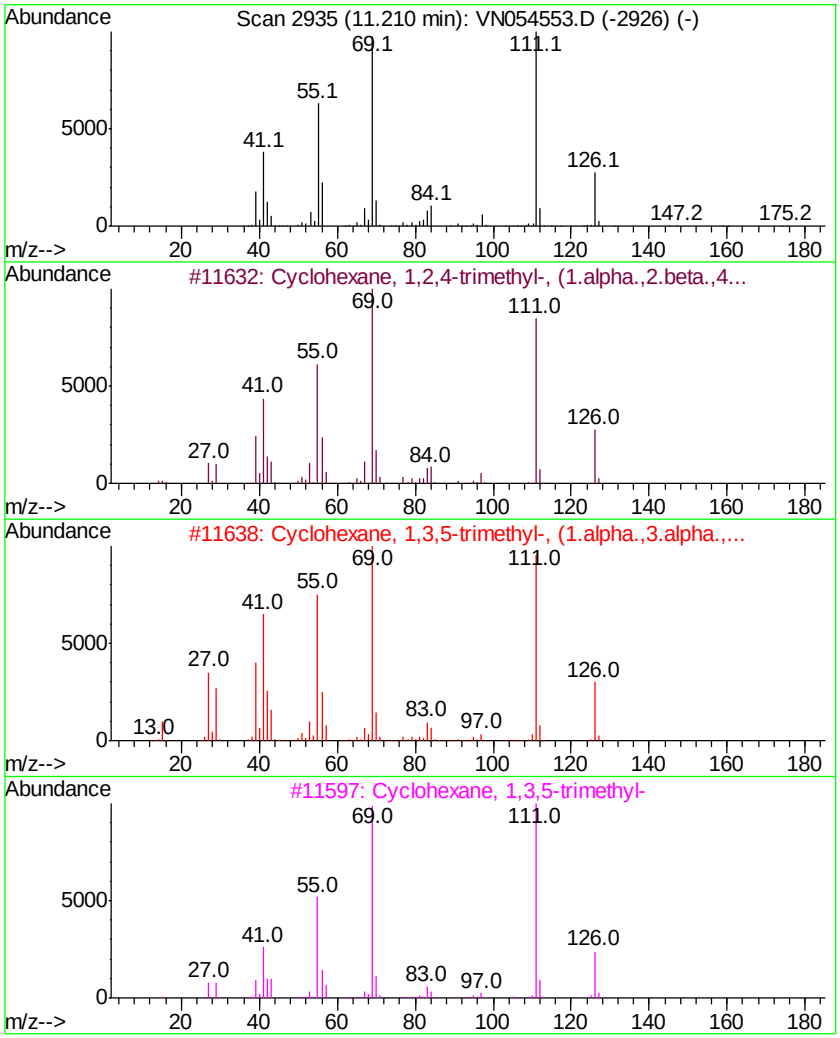
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

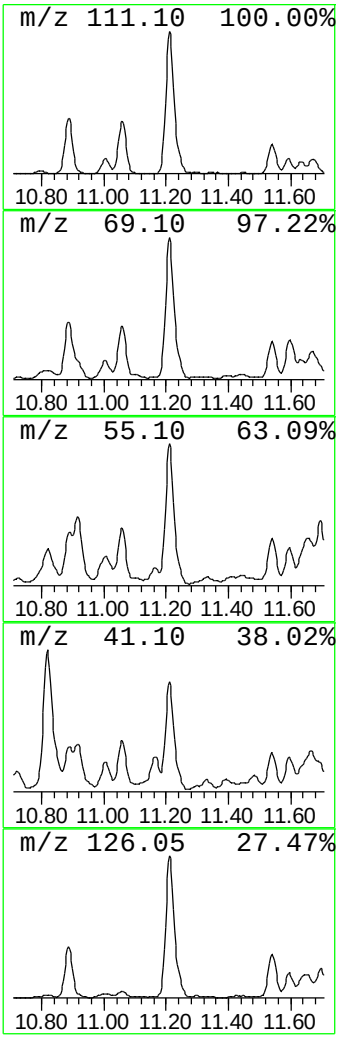
****

Peak Number 7 Cyclohexane, 1,2,4-trimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	61.11 ug/l	3092290	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	94
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	94
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	93
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	90
5	Cyclooctane, butyl-	168	C12H24	016538-93-5	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

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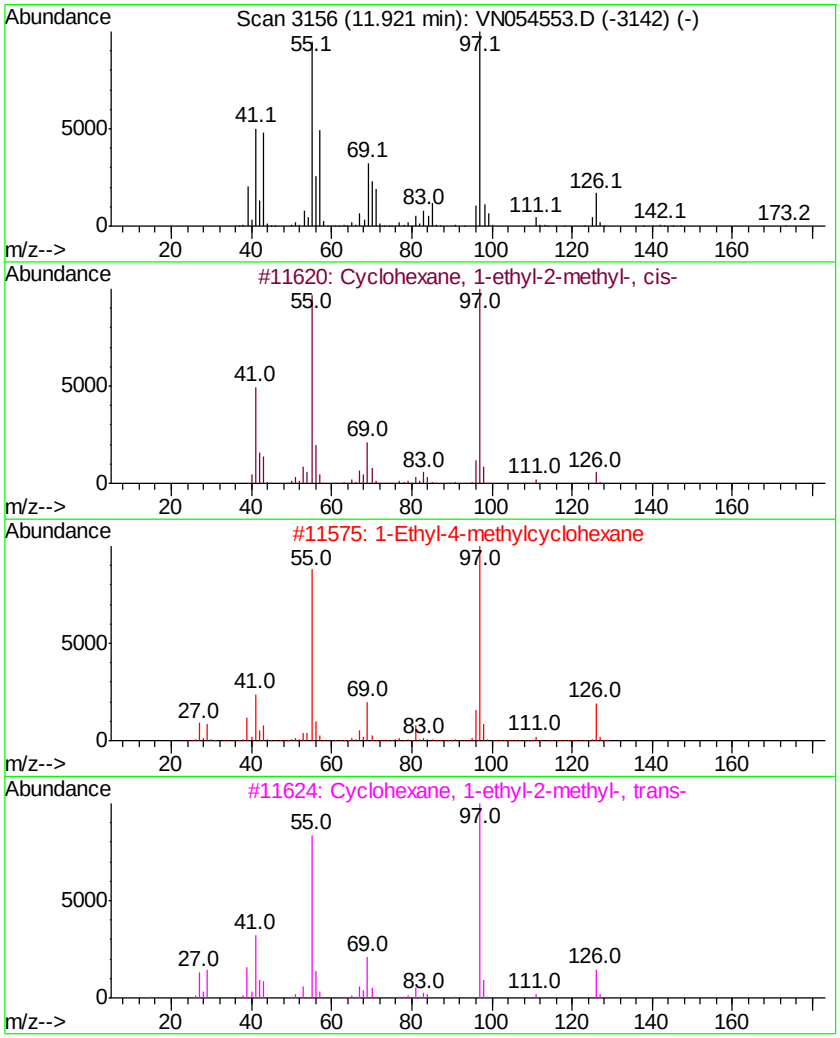
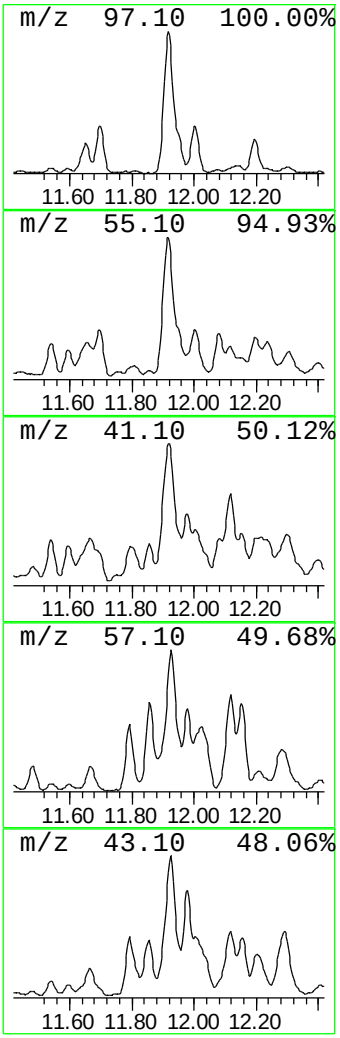
Peak Number 8 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	78.00 ug/l	3946670	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	64
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	62
3	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	62
4	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	59
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	58





Library Search Compound Report

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Data File : VN054553.D
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Operator : JC/SP
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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

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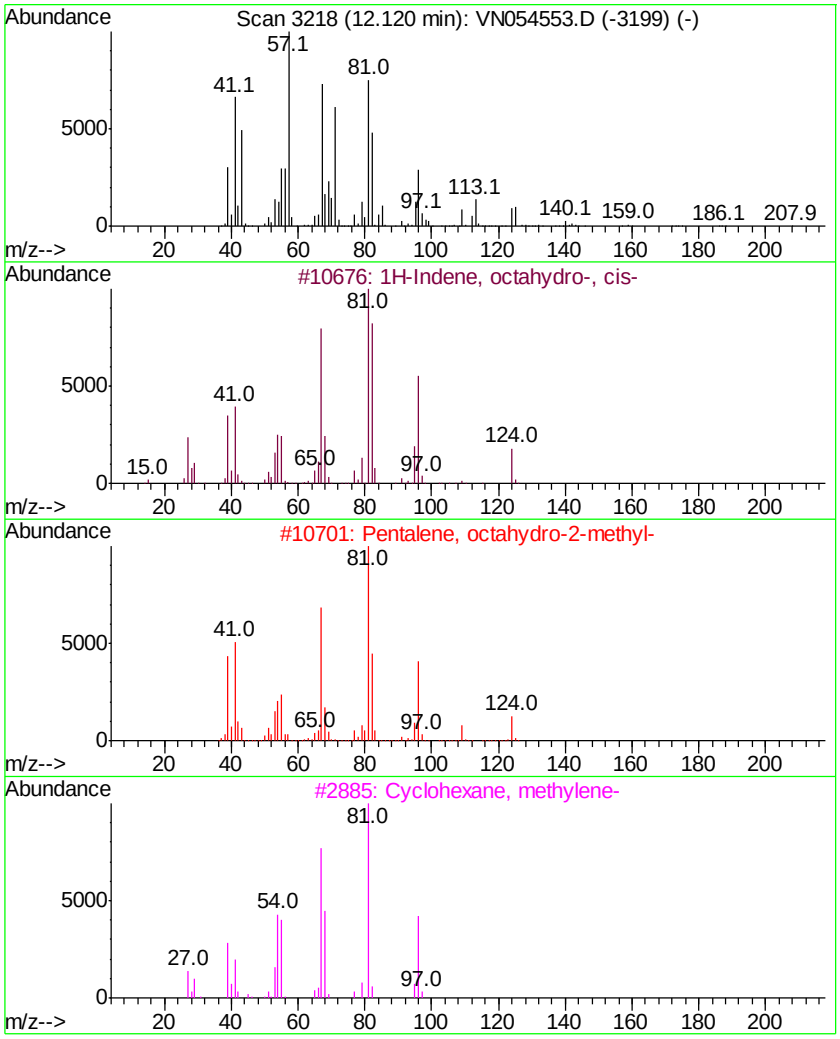
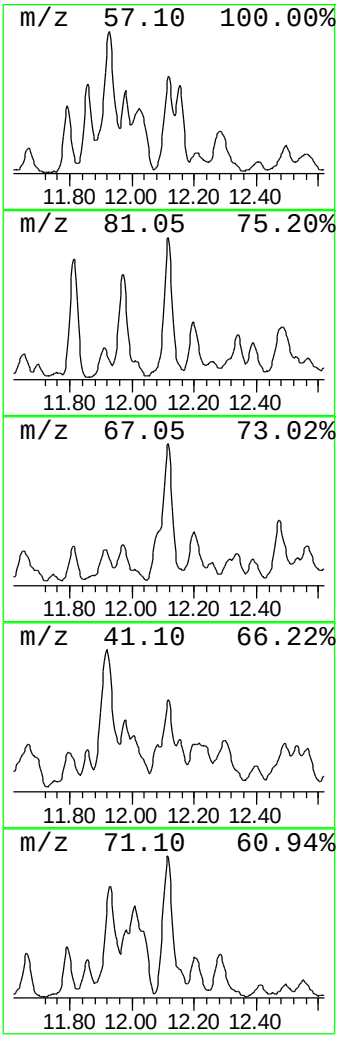
Peak Number 9 1H-Indene, octahydro-, cis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	47.55 ug/l	2406060	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	91
2	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	60
3	Cyclohexane, methylene-	96	C7H12	001192-37-6	49
4	Cyclooctene, 3-methyl-	124	C9H16	013152-05-1	46
5	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
Sample : K2004-09
Misc : 5.24g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

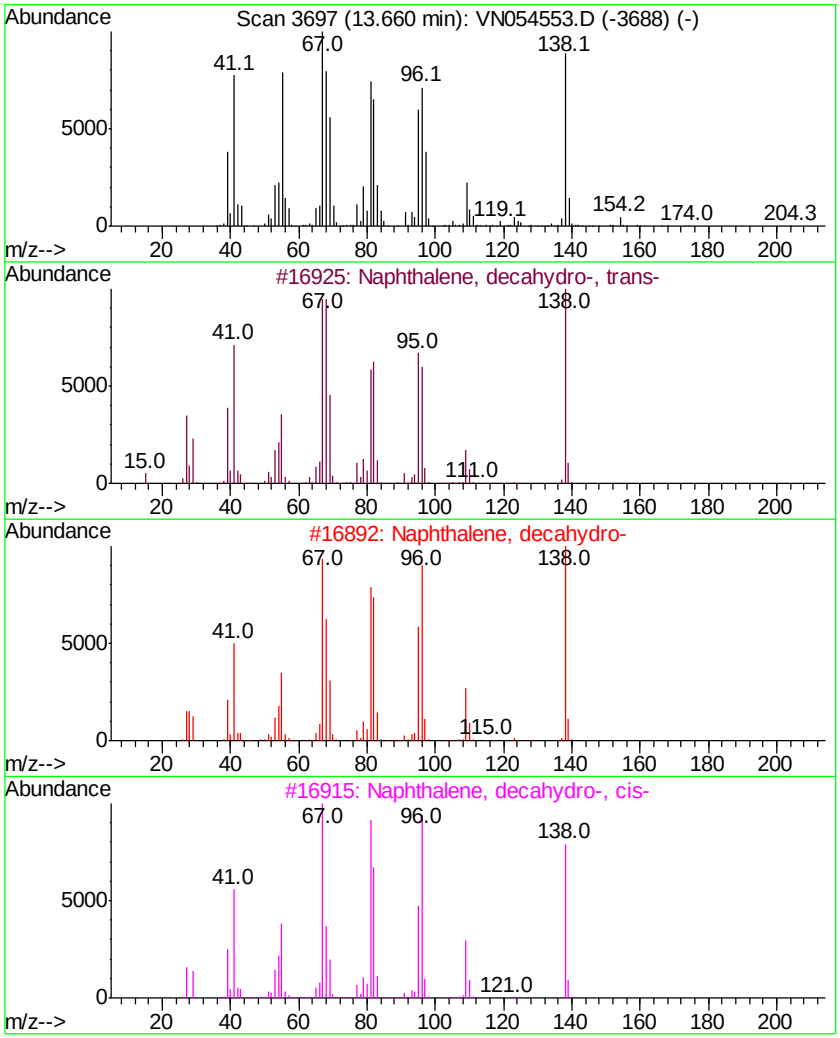
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

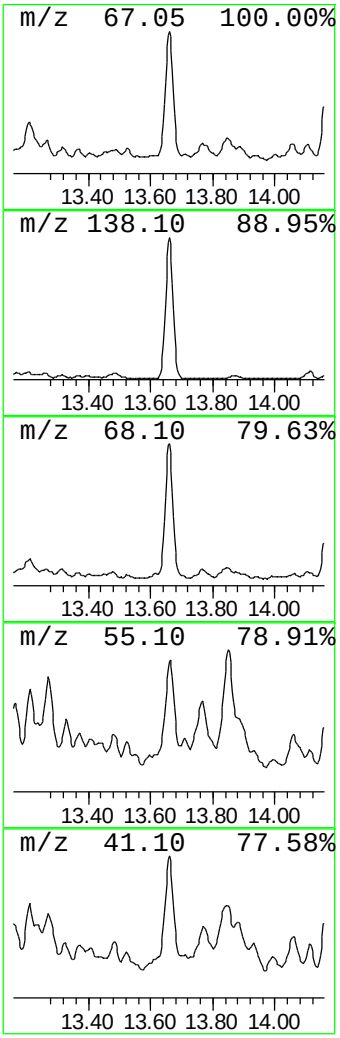
****

Peak Number 10 Naphthalene, decahydro-, tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	38.87 ug/l	1546690	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	96
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	96
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	94
4	Spiro[4.5]decane	138	C10H18	000176-63-6	81
5	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054553.D
Acq On : 22 Mar 2019 13:03
Operator : JC/SP
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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SB-22(7-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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
Pentane, 2,3-dime...	7.73	38.4	ug/l	1285890	1	7.66	1675650	50.0
Cyclopentane, 1,2...	9.36	47.2	ug/l	2165260	2	8.58	2295300	50.0
Cyclohexane, 1,1-...	10.25	33.3	ug/l	1686180	3	11.41	2529930	50.0
Cyclohexane, 1,2-...	10.43	85.2	ug/l	4310430	3	11.41	2529930	50.0
Cyclohexane, 1,4-...	10.53	35.9	ug/l	1817710	3	11.41	2529930	50.0
Heptane, 2,5-dime...	10.82	61.6	ug/l	3119160	3	11.41	2529930	50.0
Cyclohexane, 1,2,...	11.21	61.1	ug/l	3092290	3	11.41	2529930	50.0
Cyclohexane, 1-et...	11.92	78.0	ug/l	3946670	3	11.41	2529930	50.0
1H-Indene, octahy...	12.12	47.5	ug/l	2406060	3	11.41	2529930	50.0
Naphthalene, deca...	13.66	38.9	ug/l	1546690	4	13.34	1989760	50.0