LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054589.D
Acq On : 23 Mar 2019 6:28
Operator : JC/SP
Sample : K2045-15
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB436-190320-(22-24)

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	6.825	1549	1571	1595	rBV2	312091	915934	1.60%	0.322%
2	7.590	1789	1809	1818	rBV2	345941	931797	1.63%	0.327%
3	7.661	1820	1831	1846	rVB	685702	1668770	2.92%	0.586%
4	8.027	1929	1945	1966	rVB2	420713	993656	1.74%	0.349%
5	8.201	1989	1999	2017	rVB	231199	592195	1.04%	0.208%
6	8.583	2103	2118	2144	rVB	996599	2088424	3.66%	0.733%
7	9.075	2241	2271	2284	rBV2	726214	1708125	2.99%	0.600%
8	9.651	2434	2450	2462	rBV2	295139	654512	1.15%	0.230%
9	9.866	2498	2517	2540	rVB2	201862	574347	1.01%	0.202%
10	10.088	2573	2586	2604	rBV2	1764596	3575636	6.26%	1.255%
11	11.004	2862	2871	2881	rVB2	503870	866827	1.52%	0.304%
12	11.120	2895	2907	2914	rBV4	338399	639498	1.12%	0.224%
13	11.201	2915	2932	2950	rVB5	672174	1997983	3.50%	0.701%
14	11.297	2950	2962	2983	rBV	920518	1755450	3.07%	0.616%
15	11.432	2984	3004	3021	rBV	19151522	36562859	64.04%	12.834%
16	11.593	3044	3054	3060	rBV6	609883	1228357	2.15%	0.431%
17	11.651	3061	3072	3080	rVV3	1538501	3646481	6.39%	1.280%
18	11.696	3081	3086	3096	rVB3	1089835	1733617	3.04%	0.609%
19	11.850	3127	3134	3142	rVB4	676946	1019291	1.79%	0.358%
20	11.924	3143	3157	3170	rBV7	2542984	6722707	11.77%	2.360%
21	12.043	3187	3194	3201	rVB	2630050	3539075	6.20%	1.242%
22	12.117	3209	3217	3222	rBV3	1888356	2935989	5.14%	1.031%
23	12.162	3223	3231	3250	rVB4	4371001	8412158	14.73%	2.953%
24	12.294	3262	3272	3280	rVB6	1677734	3029969	5.31%	1.064%
25	12.403	3297	3306	3315	rBV5	1610133	2934726	5.14%	1.030%
26	12.561	3347	3355	3371	rVB3	3545120	7414117	12.98%	2.602%
27	12.641	3371	3380	3389	rVV5	1333641	2815941	4.93%	0.988%
28	12.728	3393	3407	3416	rVV5	5365704	13848272	24.25%	4.861%
29	12.779	3417	3423	3433	rVB2	2642262	4106060	7.19%	1.441%
30	12.869	3443	3451	3455	rBV4	1392553	2283720	4.00%	0.802%
31	12.959	3473	3479	3494	rVB5	2477865	4716355	8.26%	1.655%
32	13.165	3532	3543	3551	rVV7	1644159	3632652	6.36%	1.275%
33	13.239	3552	3566	3572	rVV3	4431995	9076602	15.90%	3.186%
34	13.284	3572	3580	3590	rVV	8157444	13843727	24.25%	4.859%

LSC Area Percent Report

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Instrument : MSVOA_N
ClientSampleId : WP022SB436-190320-(22-24)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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

35	13.364	3592	3605	3623	rVB2	25914930	45846338	80.29%	16.093%
36	13.590	3666	3675	3677	rBV3	1386663	1873267	3.28%	0.658%
37	13.654	3685	3695	3708	rVB	33079863	57098103	100.00%	20.042%
38	13.991	3789	3800	3810	rBV4	3257351	6226569	10.91%	2.186%
39	14.069	3811	3824	3831	rVV6	741793	2119949	3.71%	0.744%
40	14.178	3848	3858	3864	rBV4	2219673	4564493	7.99%	1.602%
41	14.294	3886	3894	3900	rBV3	1880308	2833775	4.96%	0.995%
42	14.332	3901	3906	3913	rVB3	1322295	1745215	3.06%	0.613%
43	14.522	3950	3965	3974	rVB4	1116780	2548452	4.46%	0.895%
44	14.577	3974	3982	3987	rBV	669408	1100620	1.93%	0.386%
45	14.850	4060	4067	4074	rBV3	1018281	1562327	2.74%	0.548%
46	14.908	4078	4085	4093	rVB	1788479	2745951	4.81%	0.964%
47	15.043	4120	4127	4136	rVB2	602834	987466	1.73%	0.347%
48	15.409	4232	4241	4258	rBV8	405246	1173518	2.06%	0.412%

Sum of corrected areas: 284891872

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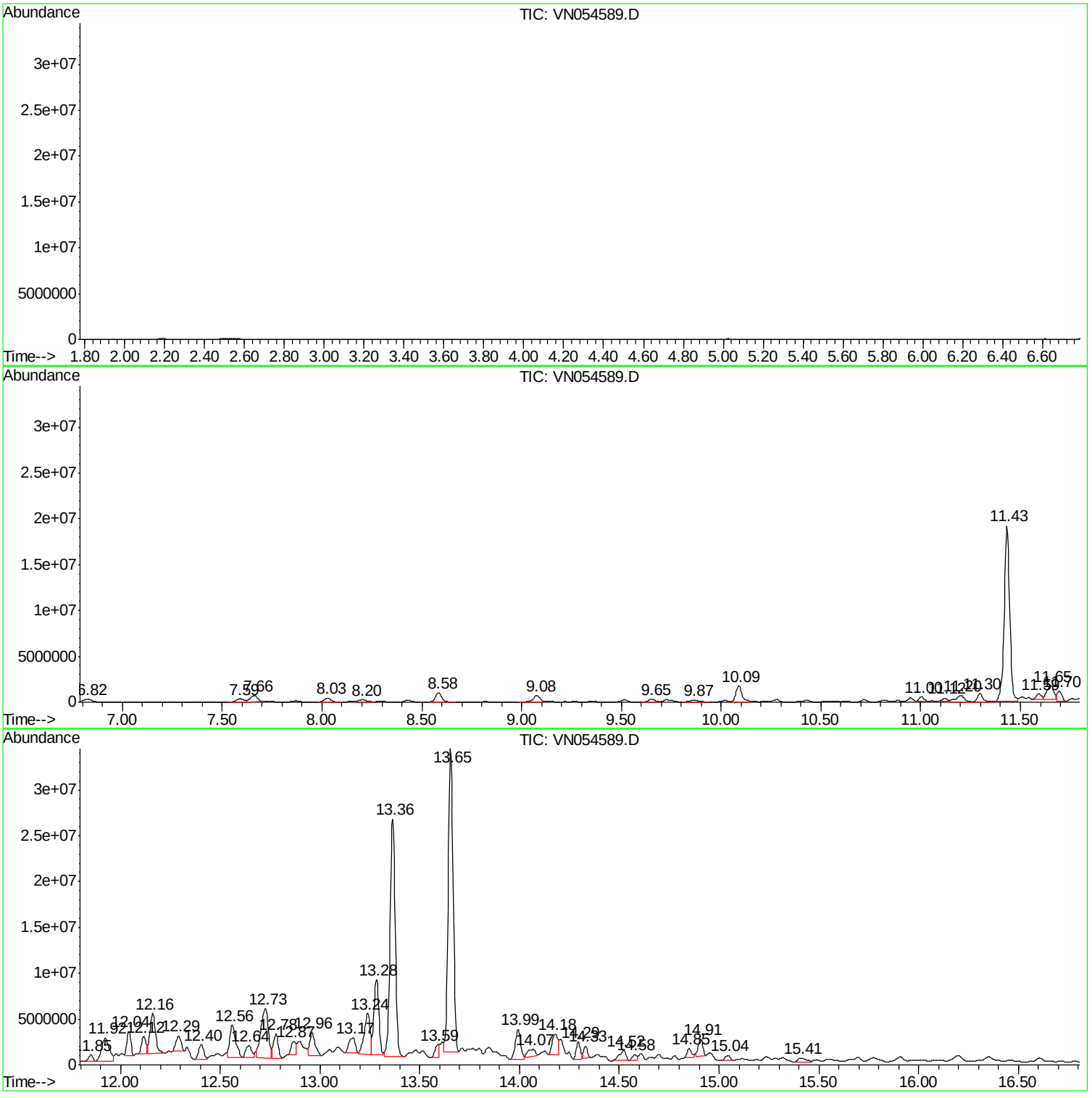
MSVOA_N
ClientSampleId :
WP022SB436-190320-(22-24)

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



Library Search Compound Report

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Quant Title : SW846 8260

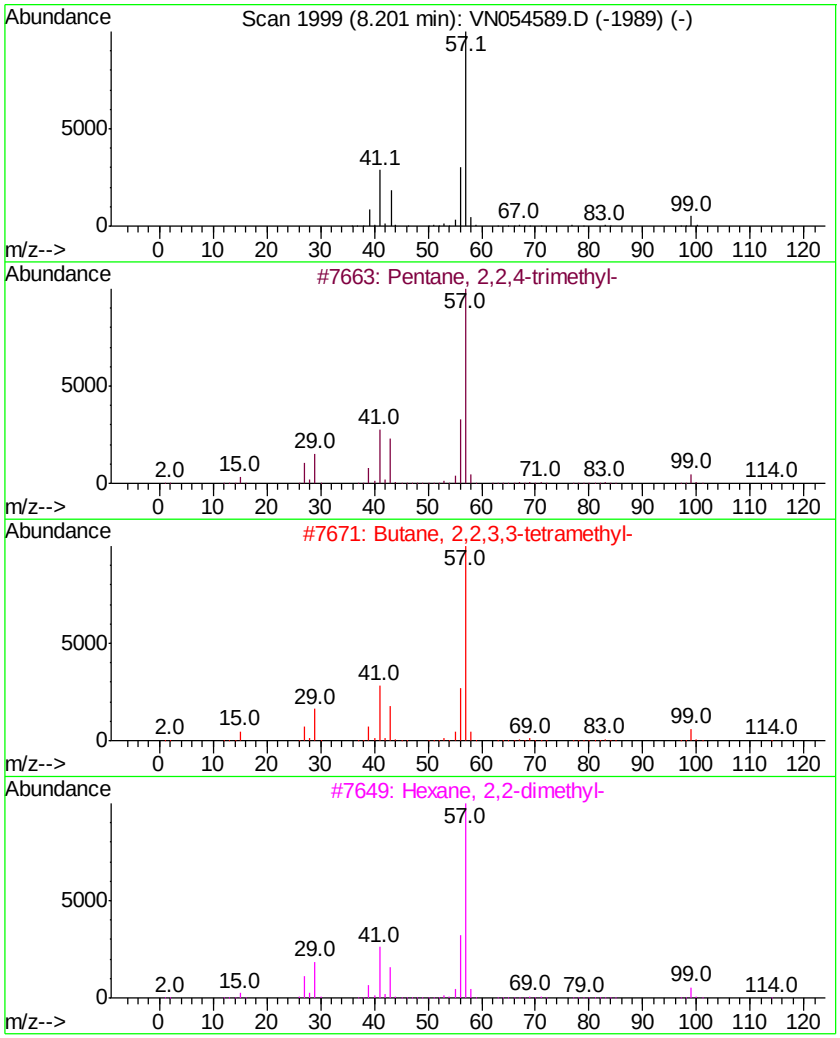
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

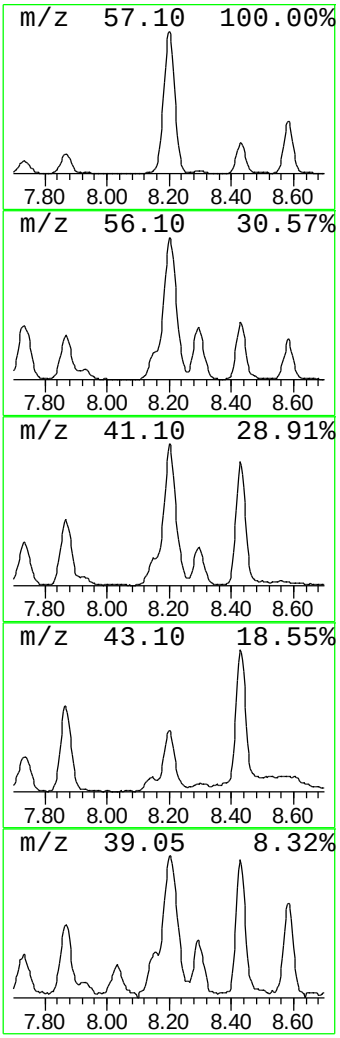
****

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	14.18 ug/l	592195	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	56
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	25





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Instrument : MSVOA_N
ClientSampleId : WP022SB436-190320-(22-24)

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

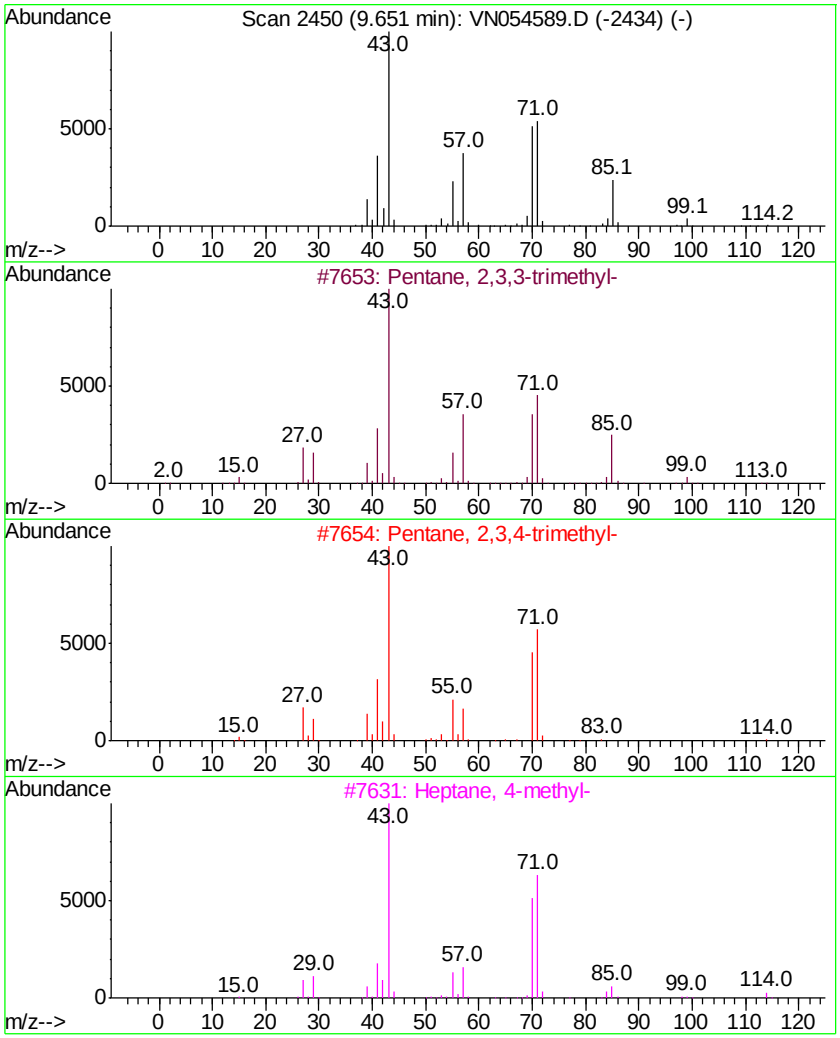
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

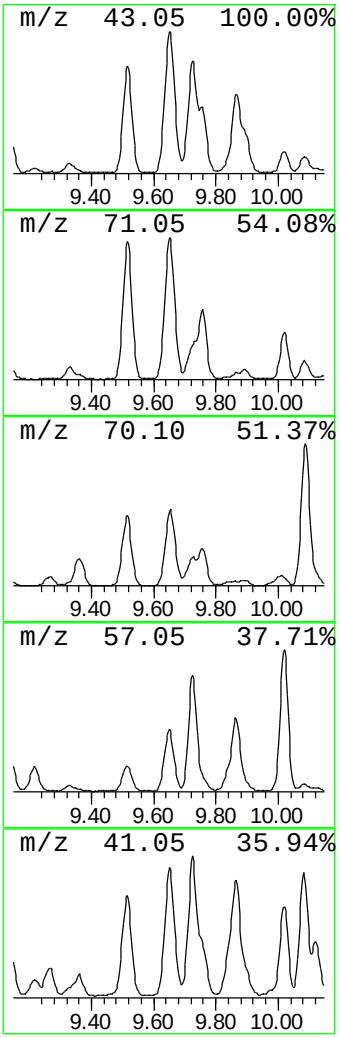
****

Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	15.67 ug/l	654512	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	68
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59





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ClientSampleId : WP022SB436-190320-(22-24)

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

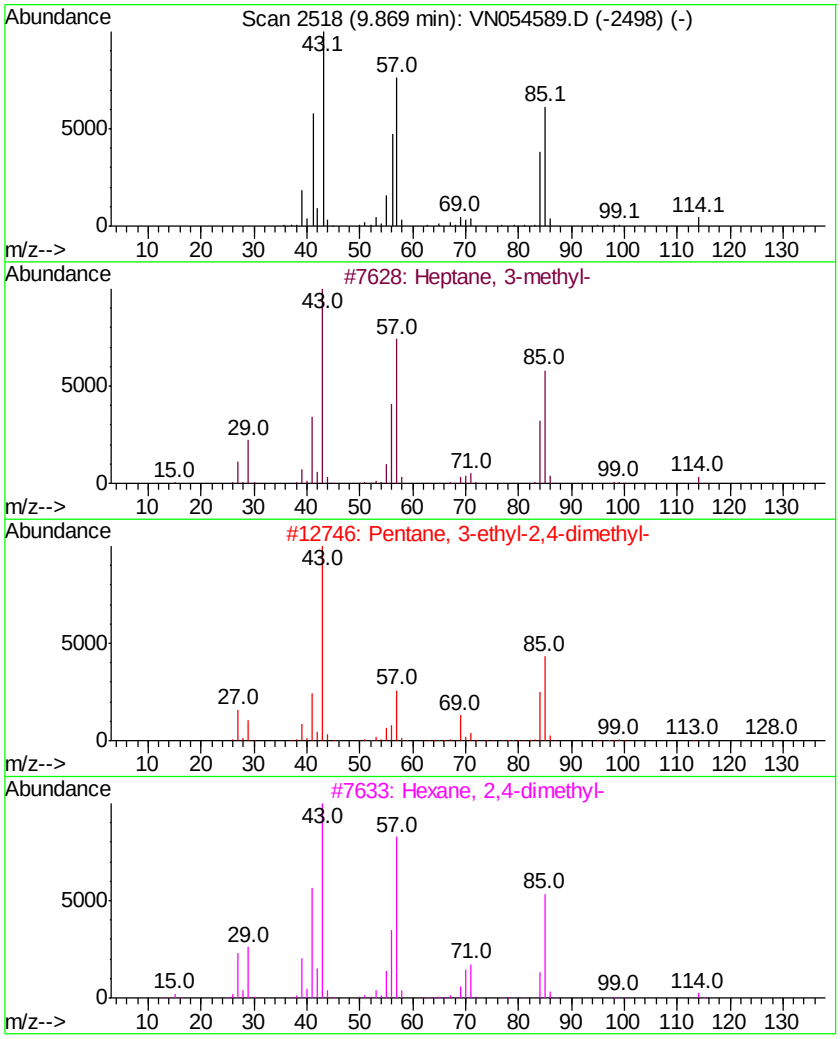
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

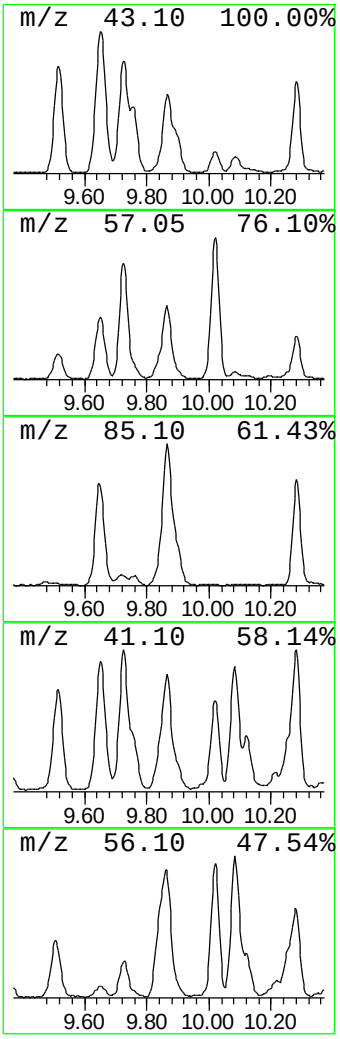
****

Peak Number 3 Heptane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	13.75 ug/l	574347	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	52
4	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	50
5	Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	50





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

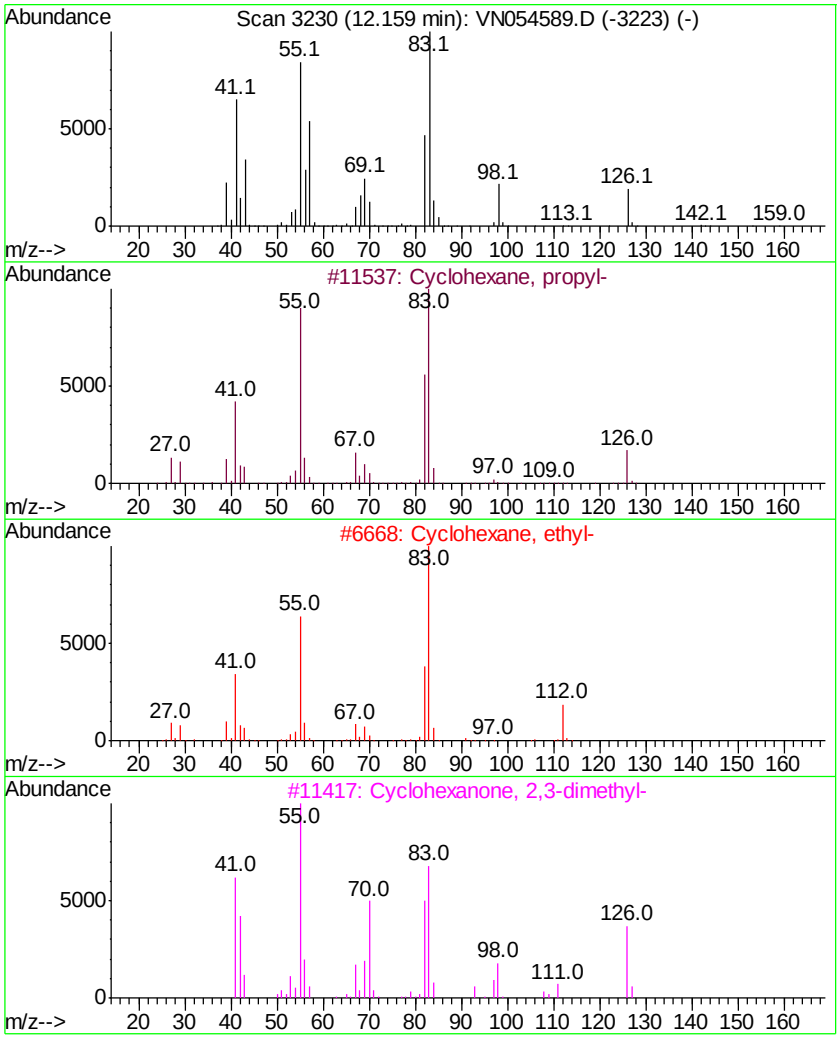
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

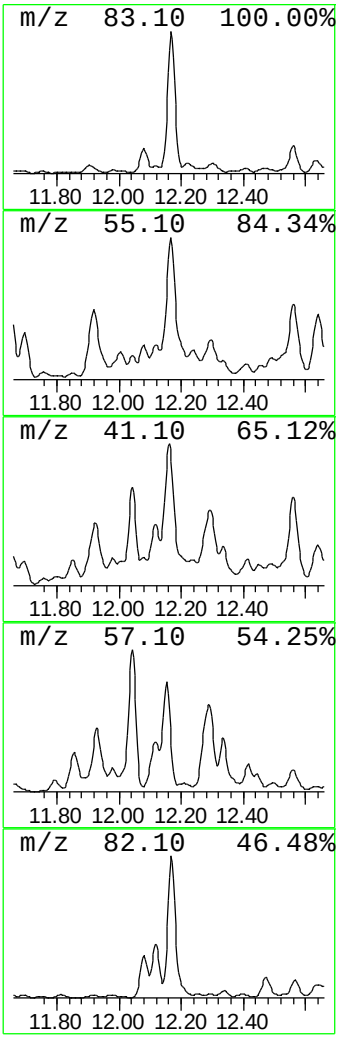
****

Peak Number 4 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	11.50 ug/l	8412160	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	74
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
3	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	53
4	1-Propenylaziridine	83	C5H9N	1000192-51-0	53
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	52





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Quant Title : SW846 8260

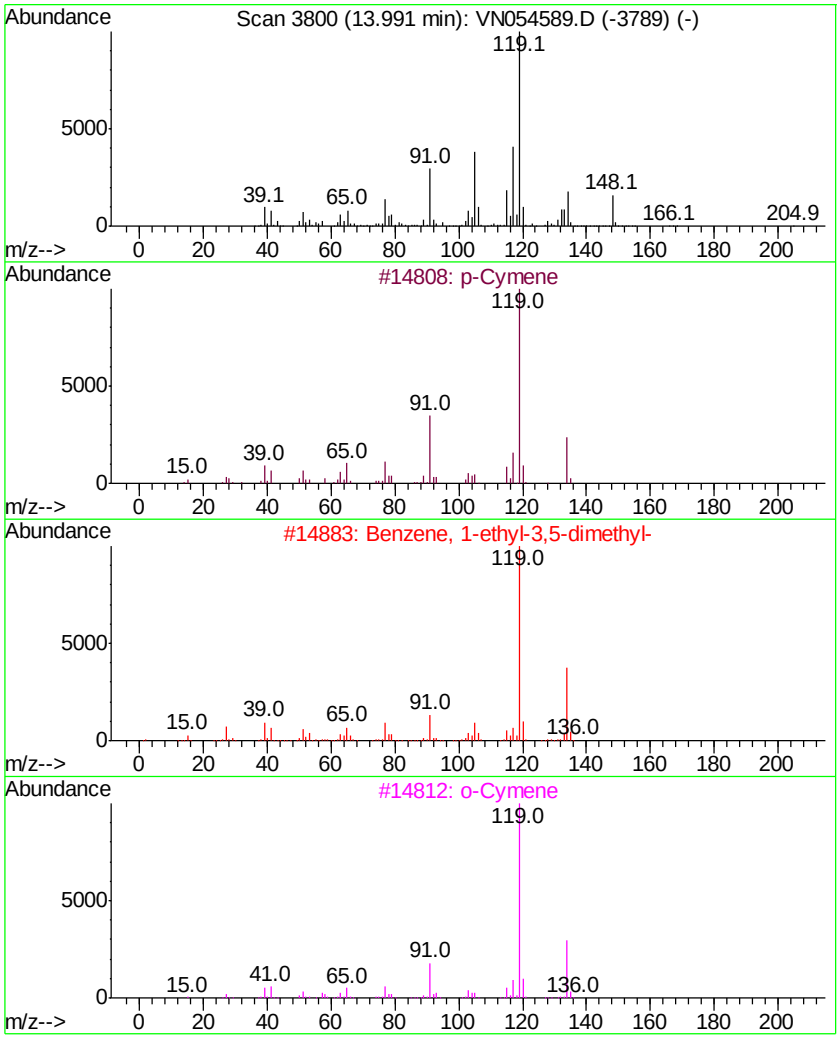
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

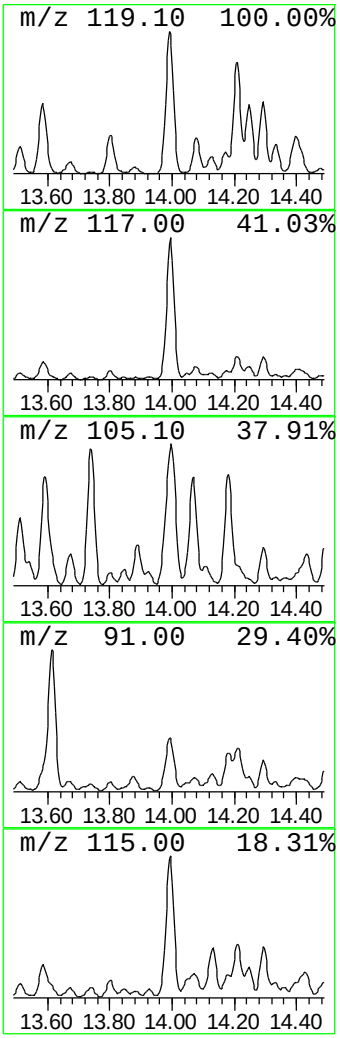
****

Peak Number 5 p-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	6.79 ug/l	6226570	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	55
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	52
3	o-Cymene	134	C10H14	000527-84-4	50
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	49
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	49





Tentatively Identified Compound (LSC) summary

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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, 2,2,4-tr...	8.20	14.2	ug/l	592195	2	8.58	2088420	50.0
Pentane, 2,3,3-tr...	9.65	15.7	ug/l	654512	2	8.58	2088420	50.0
Heptane, 3-methyl-	9.87	13.8	ug/l	574347	2	8.58	2088420	50.0
Cyclohexane, propyl-	12.16	11.5	ug/l	8412160	3	11.41	36562900	50.0
p-Cymene	13.99	6.8	ug/l	6226570	4	13.35	45846300	50.0