LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

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\82N080618W.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	1.654	3	20	47	rBV	1534600	2395247	14.28%	1.111%
2	7.593	1849	1867	1878	rBV	598227	1544604	9.21%	0.716%
3	7.667	1878	1890	1908	rVB	1009048	2436968	14.53%	1.130%
4	7.876	1942	1955	1968	rBV2	71169	171081	1.02%	0.079%
5	8.030	1988	2003	2022	rBV	612167	1422026	8.48%	0.659%
6	8.439	2119	2130	2146	rVB	224777	451840	2.69%	0.210%
7	8.587	2162	2176	2203	rBV	1382927	2887404	17.21%	1.339%
8	9.082	2320	2330	2343	rVB	424566	866701	5.17%	0.402%
9	9.728	2523	2531	2554	rVB2	291093	660033	3.93%	0.306%
10	10.091	2633	2644	2656	rBV	2758264	5083608	30.30%	2.357%
11	10.156	2659	2664	2675	rVB	472020	779921	4.65%	0.362%
12	10.284	2696	2704	2719	rVB	800500	1384806	8.25%	0.642%
13	10.718	2834	2839	2849	rVB	223249	335278	2.00%	0.155%
14	11.008	2923	2929	2940	rVB	405437	689065	4.11%	0.319%
15	11.204	2983	2990	3008	rVB8	514284	1039389	6.20%	0.482%
16	11.300	3015	3020	3042	rVB	496881	900840	5.37%	0.418%
17	11.410	3044	3054	3068	rVV	1811610	3141206	18.72%	1.456%
18	11.512	3078	3086	3097	rBV	846895	1798446	10.72%	0.834%
19	11.628	3111	3122	3139	rVB2	2820732	6826833	40.69%	3.165%
20	12.403	3356	3363	3371	rVB	1644217	2387764	14.23%	1.107%
21	12.657	3434	3442	3448	rBV	1514415	2336289	13.93%	1.083%
22	12.731	3457	3465	3475	rVB2	4995641	7644751	45.57%	3.545%
23	12.963	3531	3537	3550	rVB2	1243528	1974496	11.77%	0.915%
24	13.043	3552	3562	3571	rBV	4121878	6744011	40.20%	3.127%
25	13.239	3617	3623	3630	rVB4	1083410	1544033	9.20%	0.716%
26	13.348	3651	3657	3663	rBV2	1587255	2439436	14.54%	1.131%
27	13.541	3713	3717	3724	rVB2	1553332	1901074	11.33%	0.881%
28	13.586	3725	3731	3746	rVB4	1939560	3335374	19.88%	1.546%
29	13.673	3748	3758	3767	rBV	8321663	12848639	76.59%	5.957%
30	13.834	3804	3808	3817	rVB4	2266498	3067330	18.28%	1.422%
31	13.892	3819	3826	3834	rVB	2548349	3799481	22.65%	1.762%
32	13.998	3850	3859	3868	rBV2	2553863	4084236	24.35%	1.894%
33	14.300	3946	3953	3958	rBV3	2631718	3617809	21.57%	1.677%
34	14.336	3959	3964	3976	rVB3	2200437	2983375	17.78%	1.383%

LSC Area Percent Report

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Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

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\82N080618W.M
Title : SW846 8260

35	14.480	4003	4009	4015	rBV2	1404320	2386419	14.23%	1.106%
36	14.525	4016	4023	4032	rVB	10900044	15290478	91.14%	7.090%
37	14.586	4033	4042	4054	rBV5	5873567	13299191	79.27%	6.166%
38	14.647	4055	4061	4072	rVB2	3886508	6364135	37.94%	2.951%
39	14.853	4120	4125	4132	rBV3	2066391	2646047	15.77%	1.227%
40	14.963	4150	4159	4169	rBV4	2925509	5834711	34.78%	2.705%
41	15.123	4200	4209	4224	rVB2	4453554	11165933	66.56%	5.177%
42	15.245	4241	4247	4255	rVB4	2179857	3205992	19.11%	1.486%
43	15.336	4267	4275	4289	rVB2	8495454	14354569	85.57%	6.656%
44	15.422	4292	4302	4315	rBV4	2285850	6108042	36.41%	2.832%
45	16.036	4488	4493	4502	rVB2	1214280	1572791	9.38%	0.729%
46	16.165	4523	4533	4545	rBV	8883766	16776213	100.00%	7.778%
47	16.236	4550	4555	4566	rVB	3814460	6029941	35.94%	2.796%
48	16.355	4581	4592	4616	rVB2	6042513	15117403	90.11%	7.009%

Sum of corrected areas: 215675259

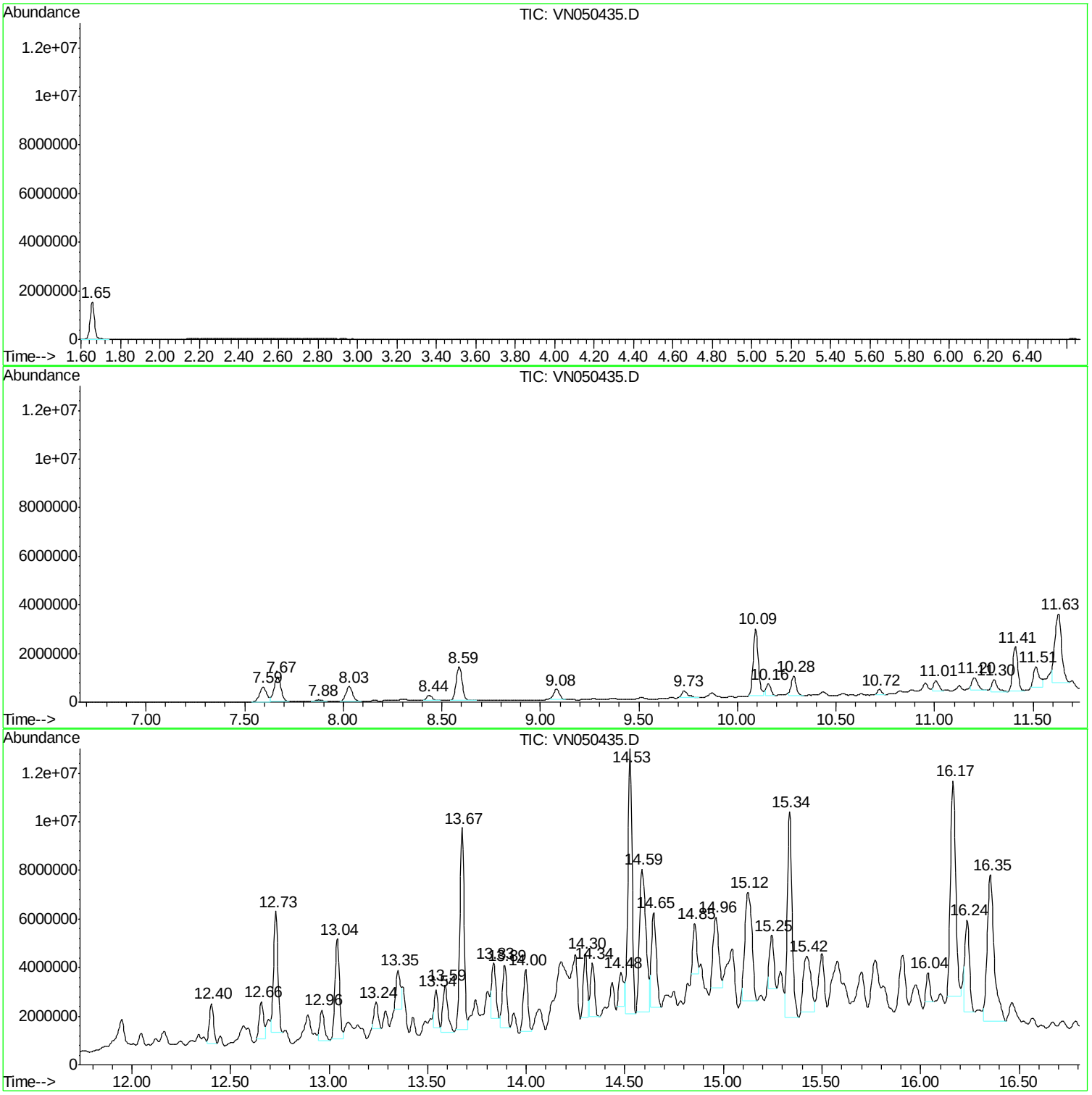
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.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\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

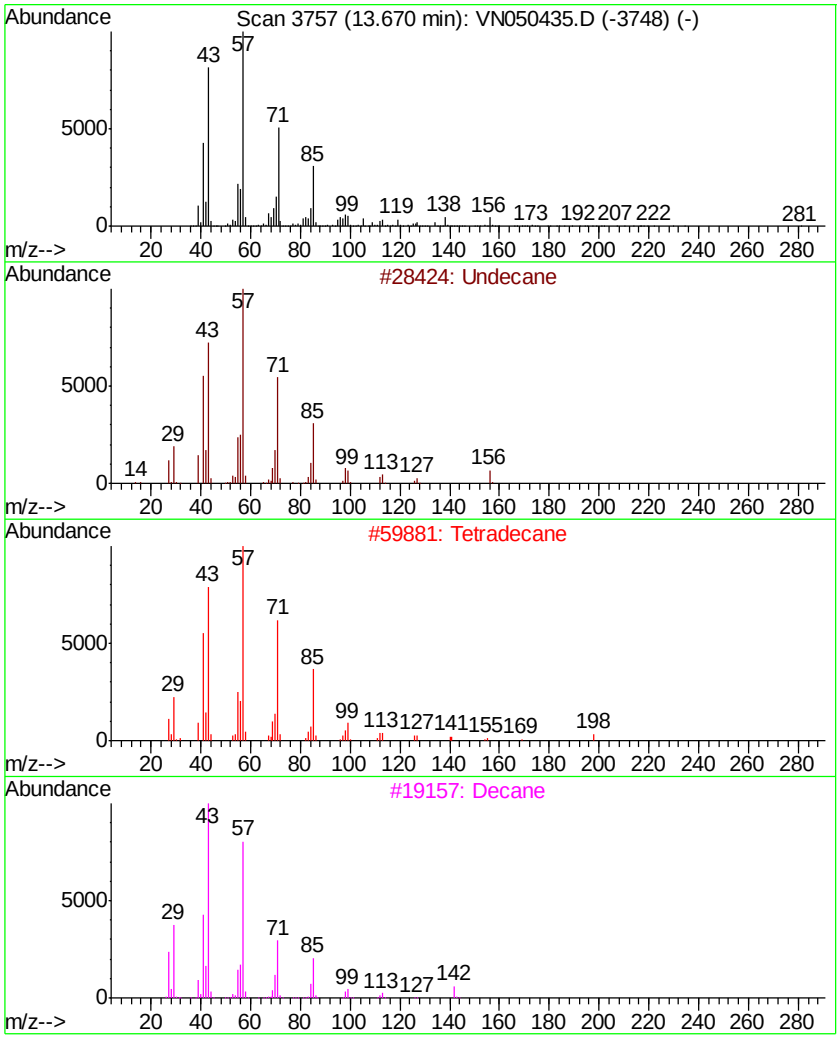
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

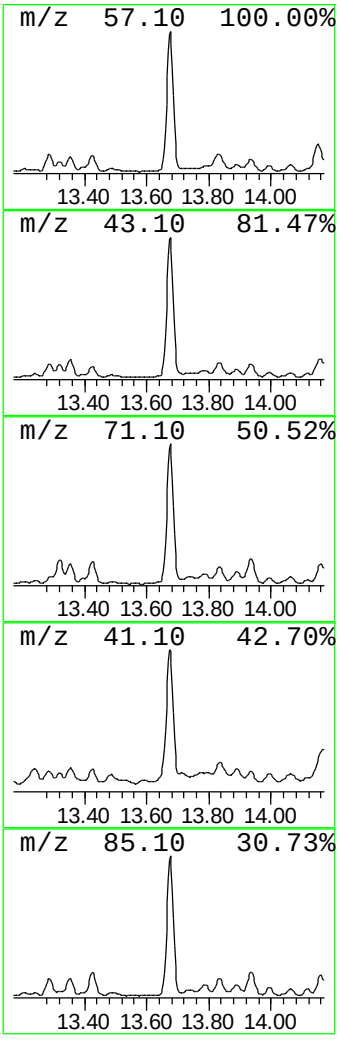
****

Peak Number 1 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	263.35 ug/l	12848600	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Tetradecane	198	C14H30	000629-59-4	90
3	Decane	142	C10H22	000124-18-5	90
4	Hexadecane	226	C16H34	000544-76-3	80
5	Dodecane	170	C12H26	000112-40-3	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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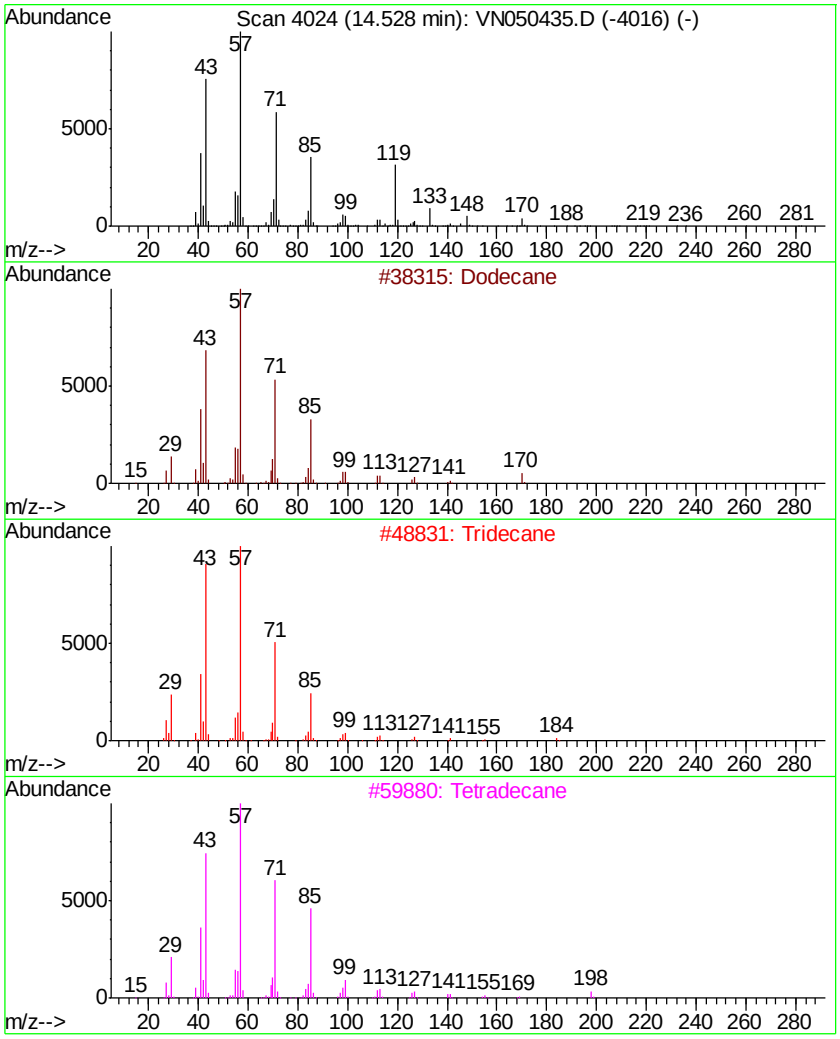
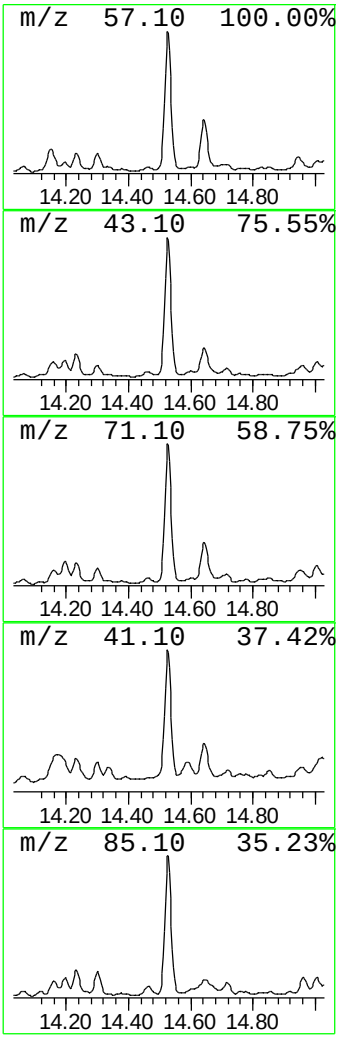
Peak Number 2 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	313.40 ug/l	15290500	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Tridecane	184	C13H28	000629-50-5	58
3	Tetradecane	198	C14H30	000629-59-4	58
4	Hexadecane	226	C16H34	000544-76-3	52
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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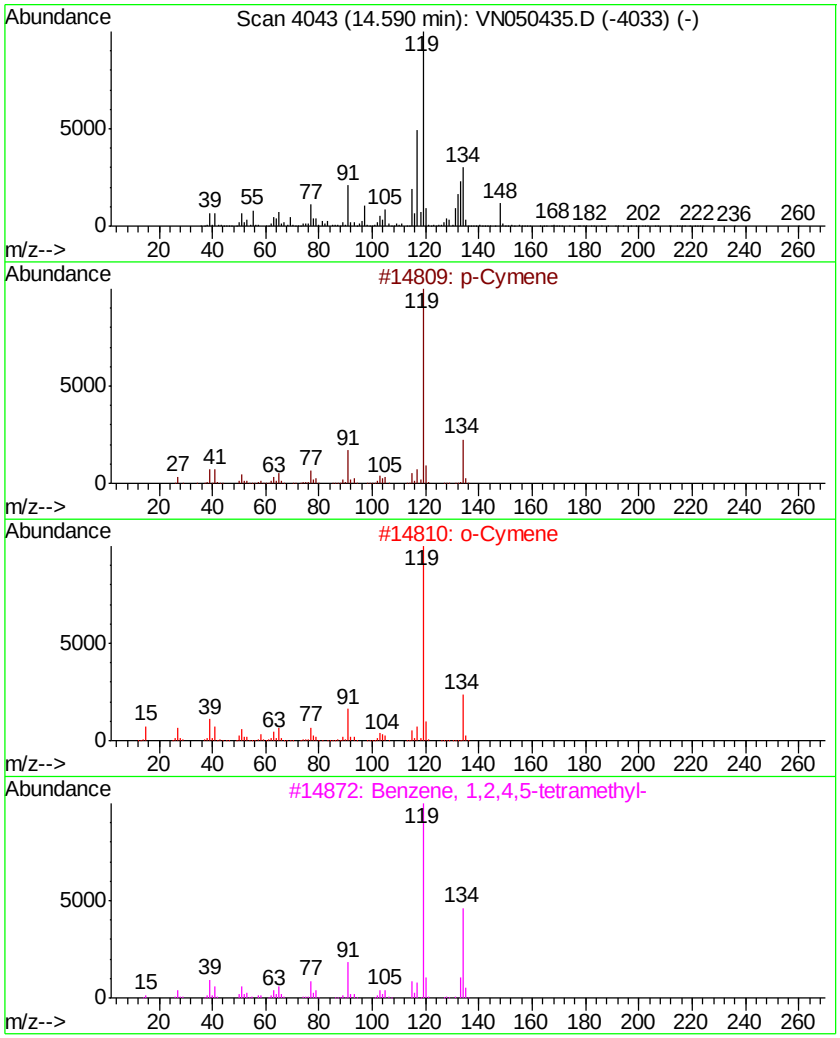
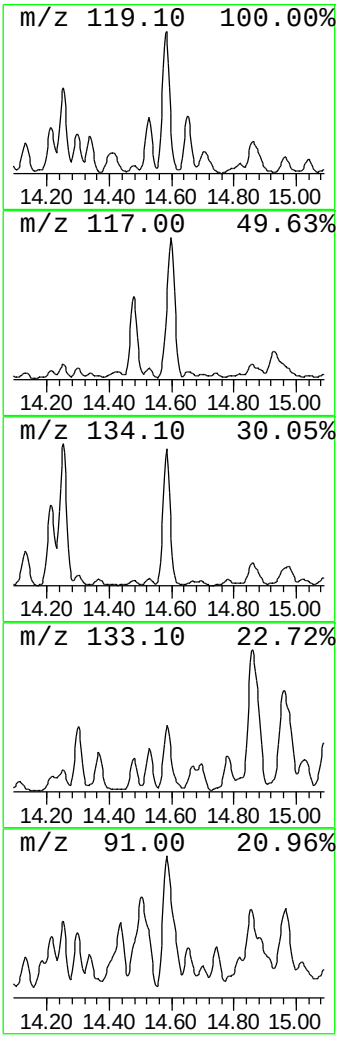
Peak Number 3 p-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	272.59 ug/l	13299200	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	64
2	o-Cymene	134	C10H14	000527-84-4	64
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	60





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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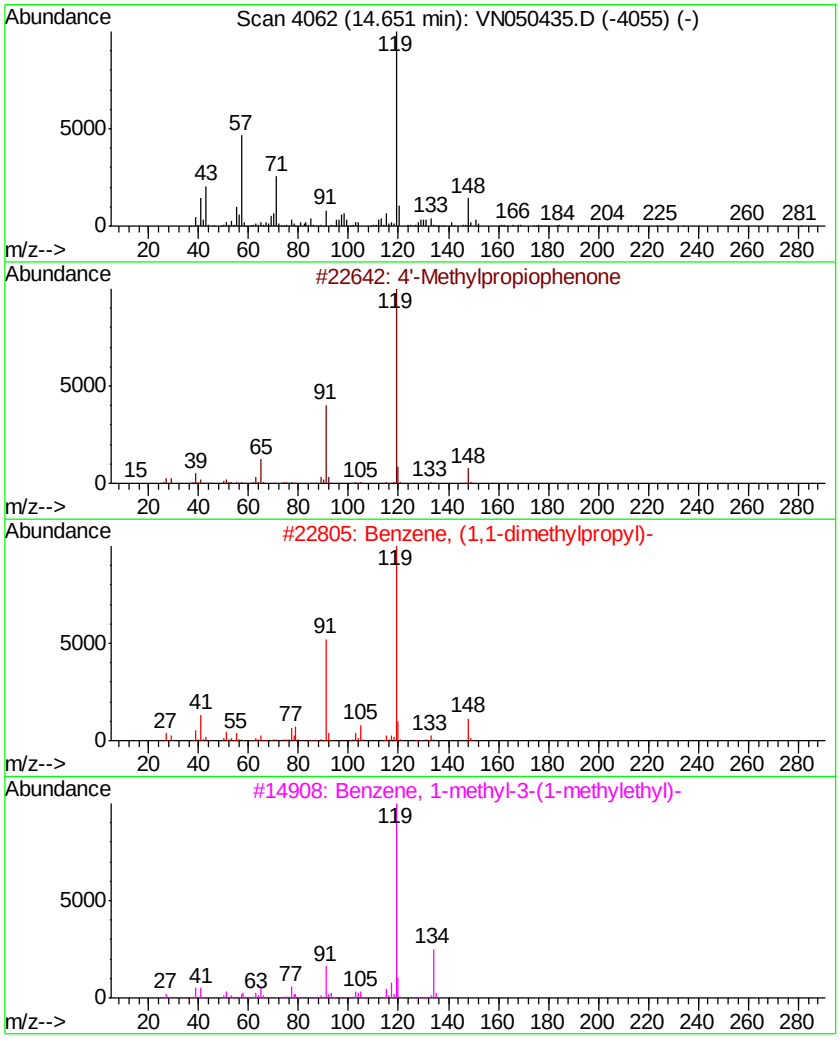
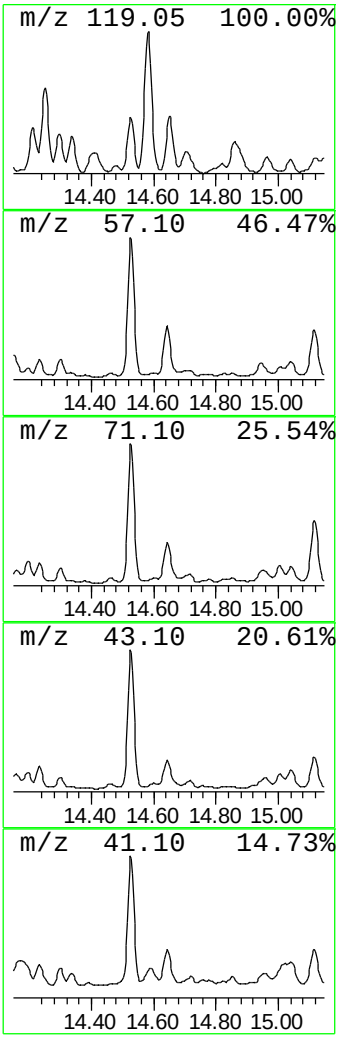
Peak Number 4 4'-Methylpropiophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	130.44 ug/l	6364140	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Methylpropiophenone	148	C10H12O	005337-93-9	50
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	50
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	43
4	p-Menthane, 2,3-dibromo-8-phenyl-	372	C16H22Br2	1000152-61-6	43
5	Dodecane, 6-methyl-	184	C13H28	006044-71-9	25





Library Search Compound Report

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Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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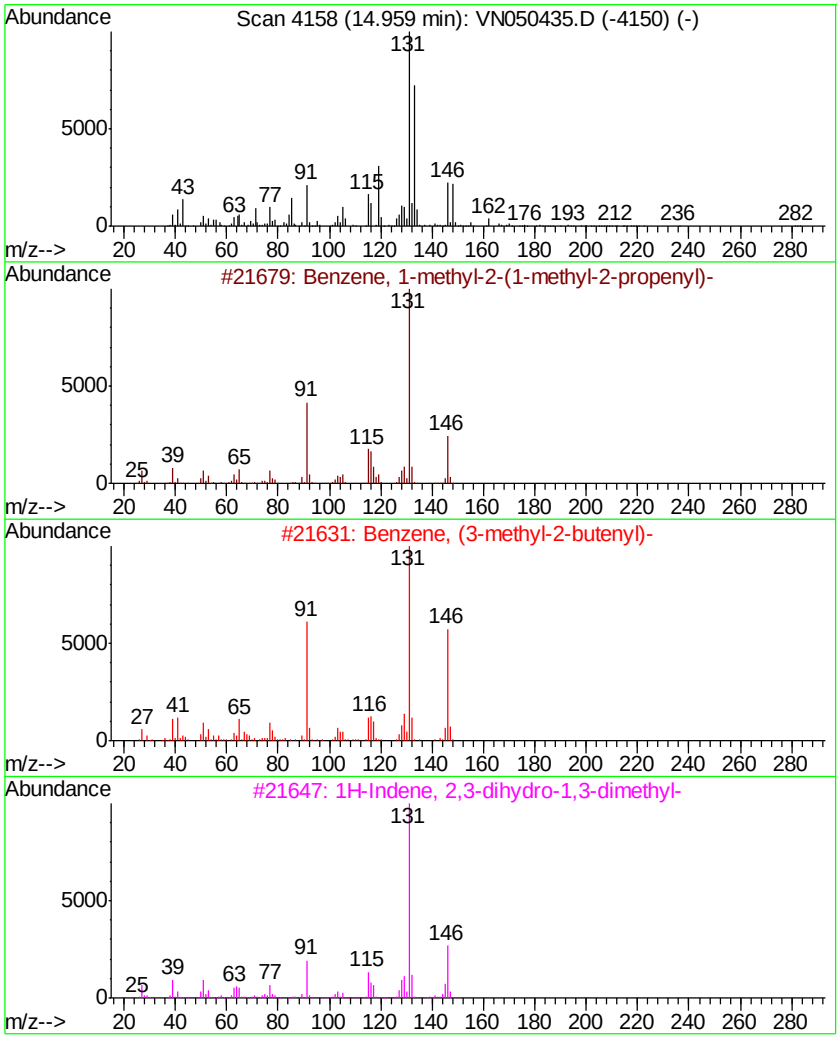
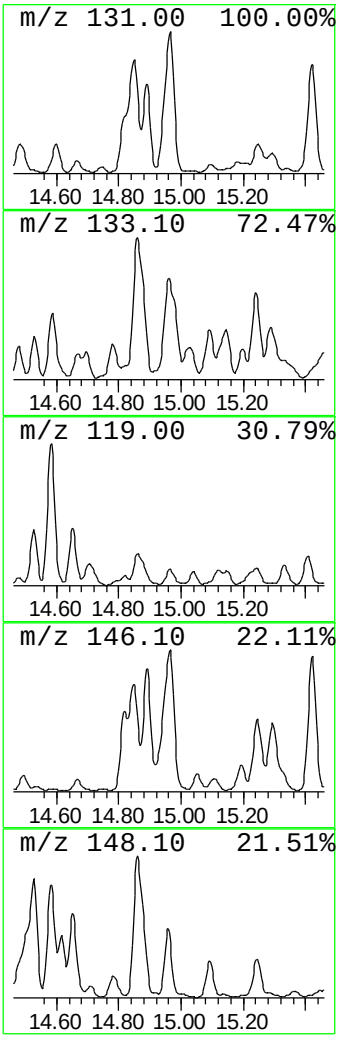
Peak Number 5 Benzene, 1-methyl-2-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	119.59 ug/l	5834710	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	64
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	60
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60
5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	60





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Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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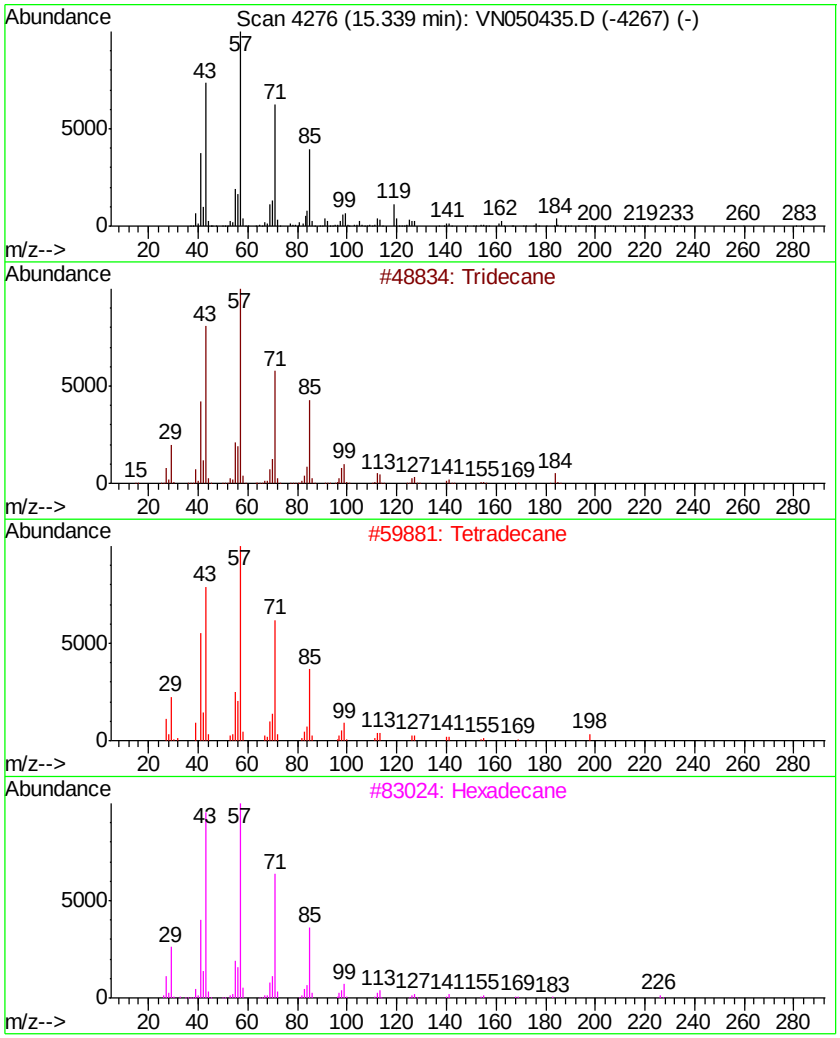
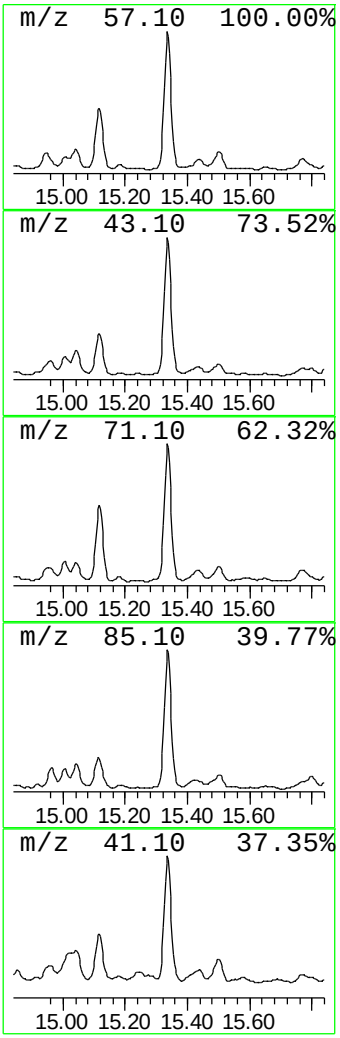
Peak Number 6 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	294.22 ug/l	14354600	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	95
2	Tetradecane	198	C14H30	000629-59-4	80
3	Hexadecane	226	C16H34	000544-76-3	74
4	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	72
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64





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Operator : MD\SY
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Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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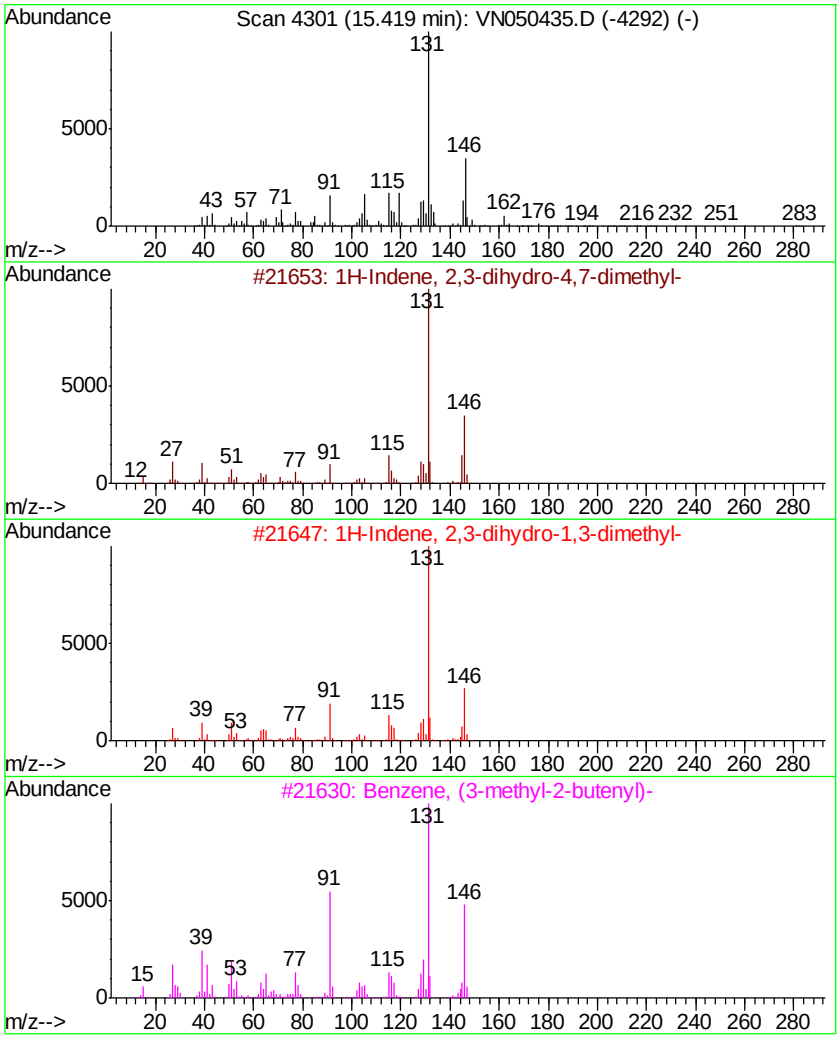
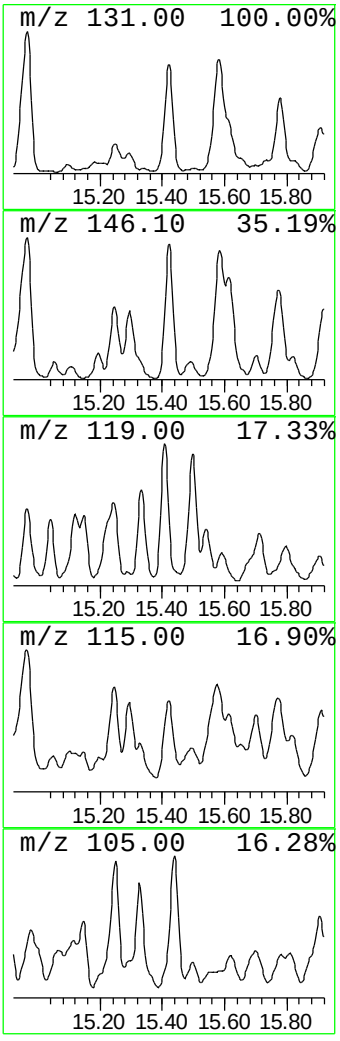
Peak Number 7 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	125.19 ug/l	6108040	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	96
2	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	90
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	90
4	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	90
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	90





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

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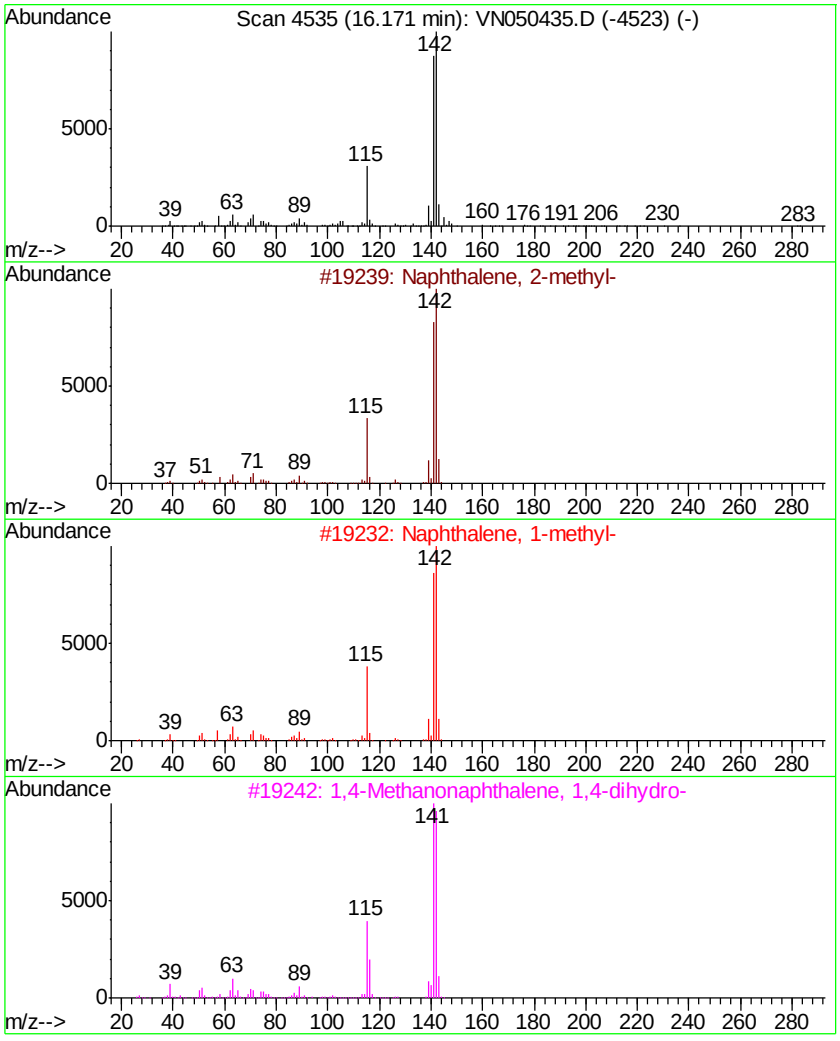
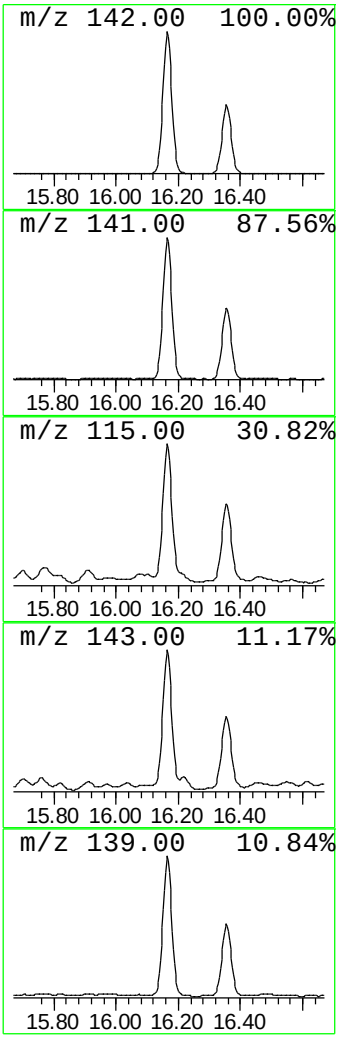
Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	343.85 ug/l	16776200	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

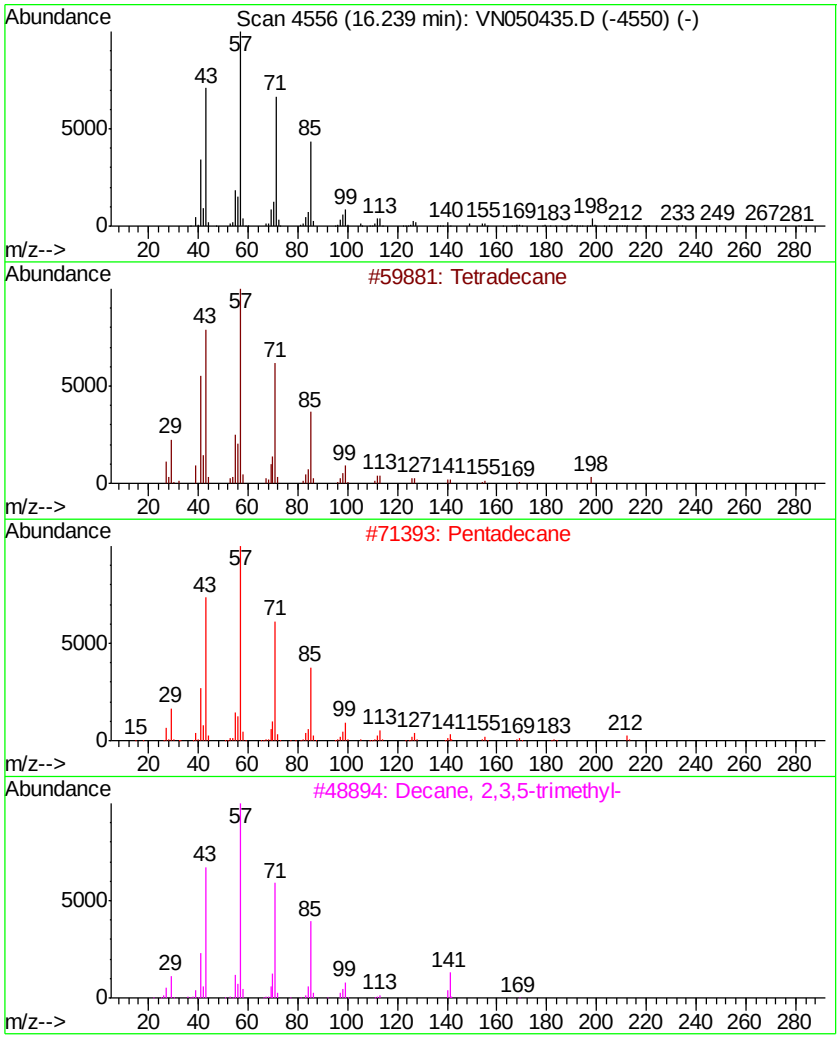
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

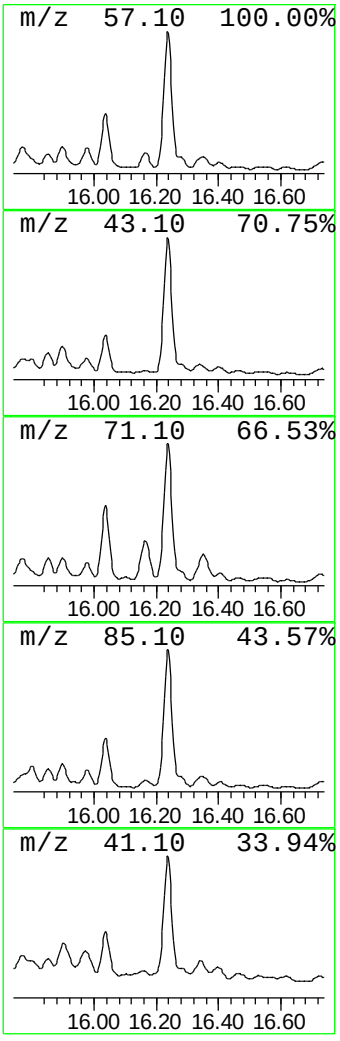
****

Peak Number 9 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	123.59 ug/l	6029940	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	94
2	Pentadecane	212	C15H32	000629-62-9	87
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4	Tridecane	184	C13H28	000629-50-5	86
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050435.D
Acq On : 7 Aug 2018 16:40
Operator : MD\SY
Sample : J4297-03 5X
Misc : 6.14g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.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
Undecane	13.67	263.4	ug/l	12848600	4	13.35	2439440	50.0
Dodecane	14.53	313.4	ug/l	15290500	4	13.35	2439440	50.0
p-Cymene	14.59	272.6	ug/l	13299200	4	13.35	2439440	50.0
4'-Methylpropioph...	14.65	130.4	ug/l	6364140	4	13.35	2439440	50.0
Benzene, 1-methyl...	14.96	119.6	ug/l	5834710	4	13.35	2439440	50.0
Tridecane	15.34	294.2	ug/l	14354600	4	13.35	2439440	50.0
1H-Indene, 2,3-di...	15.42	125.2	ug/l	6108040	4	13.35	2439440	50.0
Naphthalene, 1-me...	16.17	343.9	ug/l	16776200	4	13.35	2439440	50.0
Tetradecane	16.24	123.6	ug/l	6029940	4	13.35	2439440	50.0