LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070628.D
Acq On : 14 Jan 2022 17:20
Operator : JC/MD
Sample : N1141-05
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41172

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.304	834	863	939	rBV	6931881	24758519	17.79%	9.361%
2	7.825	2150	2176	2202	rBV5	484318	1429315	1.03%	0.540%
3	8.056	2224	2262	2285	rBV3	5723653	17040965	12.24%	6.443%
4	8.161	2286	2301	2324	rVV	1875603	4719831	3.39%	1.785%
5	8.284	2325	2347	2385	rVV	7833033	18334308	13.17%	6.932%
6	8.432	2386	2402	2424	rVV	805038	1902358	1.37%	0.719%
7	8.547	2425	2445	2463	rVV4	1102181	2852387	2.05%	1.078%
8	8.818	2526	2546	2581	rVV	8224724	16717523	12.01%	6.321%
9	8.963	2583	2600	2630	rVB	1475376	3134964	2.25%	1.185%
10	9.453	2750	2783	2795	rBV2	1534476	3857313	2.77%	1.458%
11	10.440	3133	3151	3160	rBV	2619498	4936332	3.55%	1.866%
12	10.505	3160	3175	3207	rVB3	65571017	139193501	100.00%	52.629%
13	11.746	3621	3638	3660	rBV	1828497	3292370	2.37%	1.245%
14	11.953	3700	3715	3738	rBV3	1126791	2155774	1.55%	0.815%
15	12.733	3994	4006	4030	rVB2	2072343	3860844	2.77%	1.460%
16	13.047	4112	4123	4139	rVB2	2016158	3480628	2.50%	1.316%
17	13.675	4347	4357	4376	rVB2	2130227	3581362	2.57%	1.354%
18	13.994	4464	4476	4488	rBV	3047164	4615292	3.32%	1.745%
19	14.844	4784	4793	4808	rVB2	2016858	3037745	2.18%	1.149%
20	15.702	5106	5113	5133	rVB2	840213	1578754	1.13%	0.597%

Sum of corrected areas: 264480085

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ClientSampleId :
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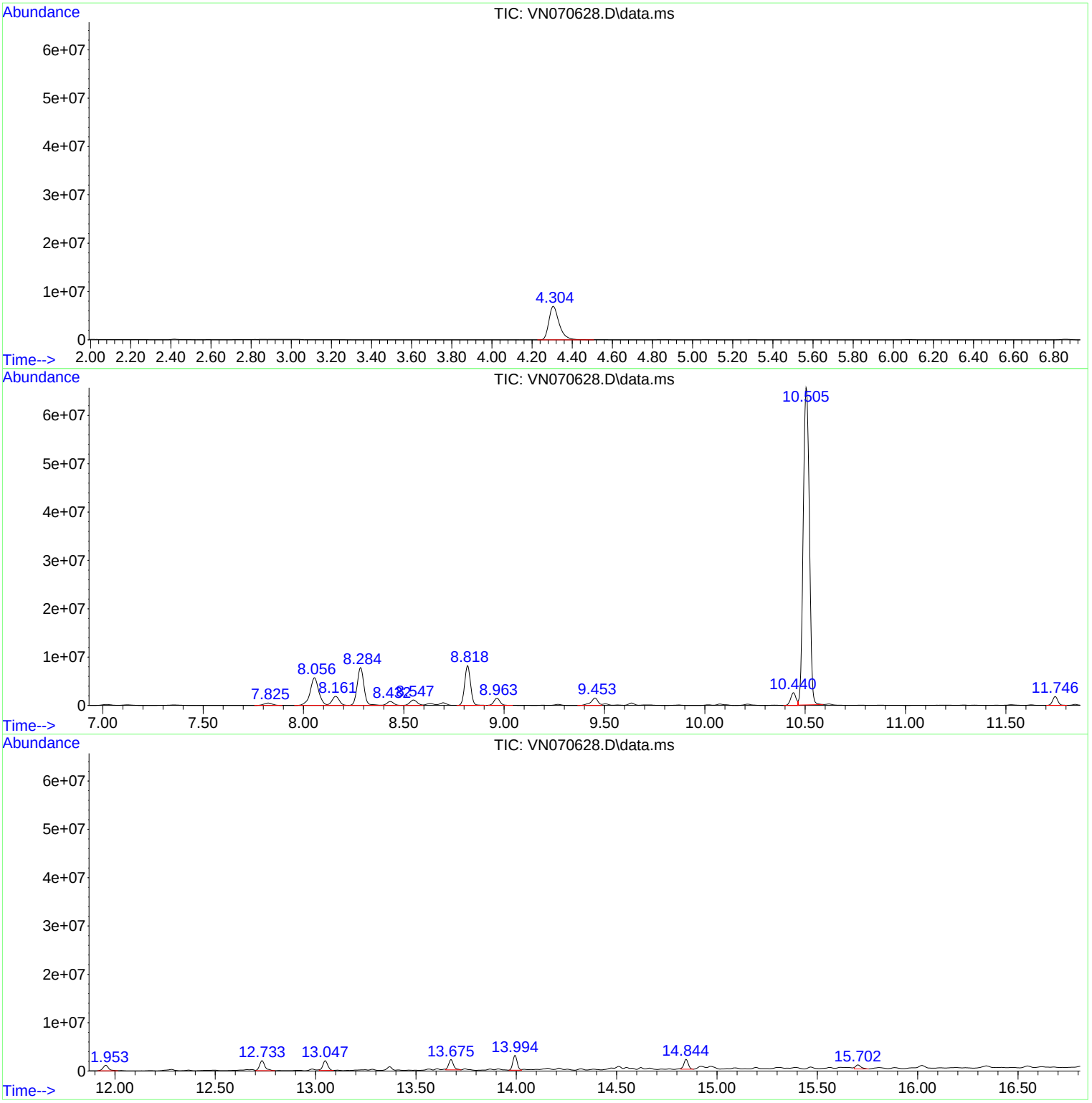
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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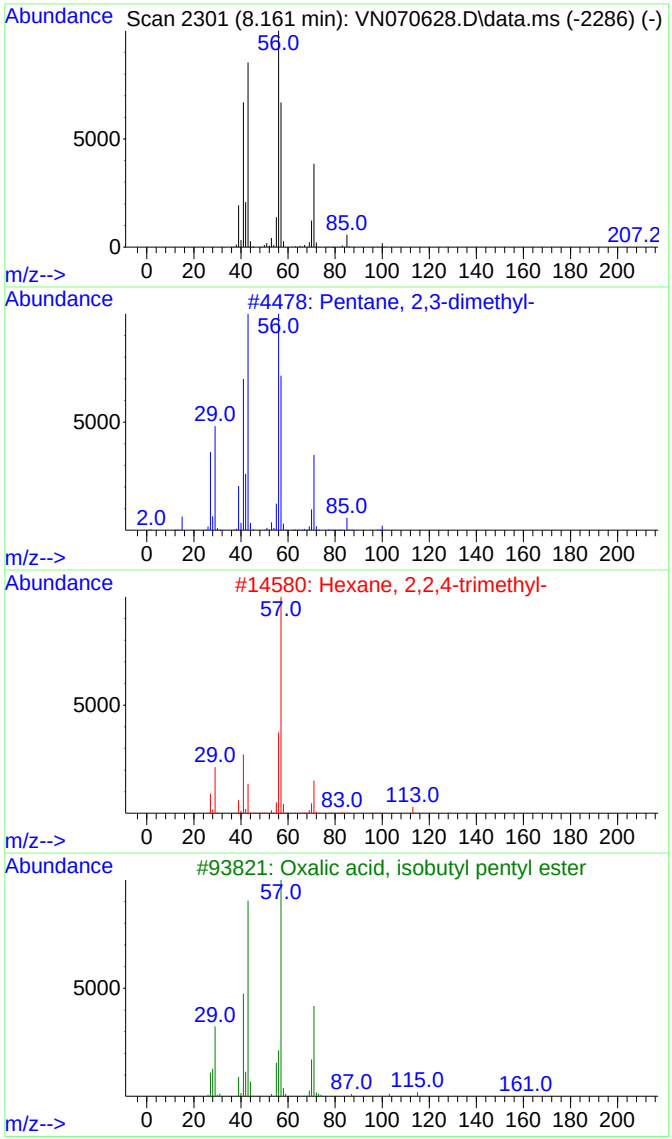
Quant Title : SW846 8260

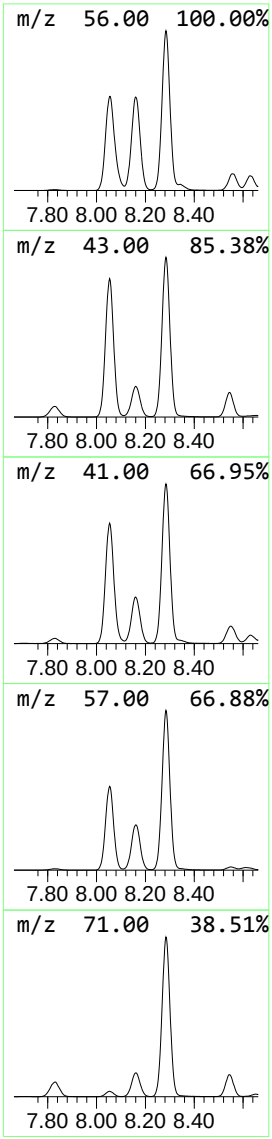
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	13.85 ug/l	4719830	Pentafluorobenzene	8.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
3	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	38
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	37





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Instrument :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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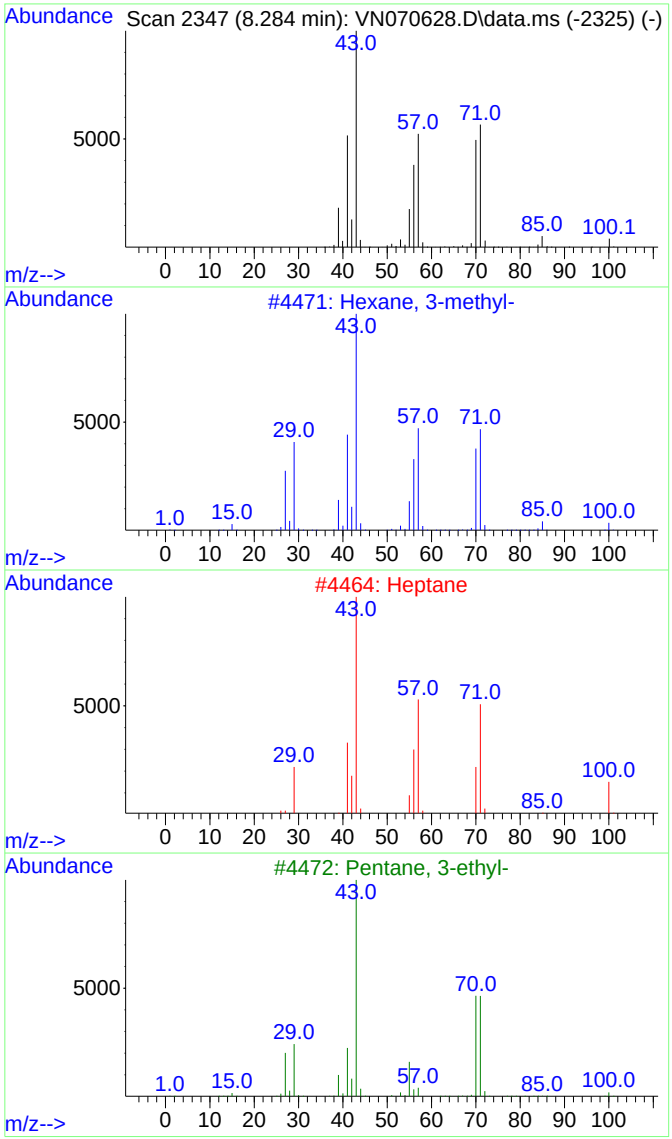
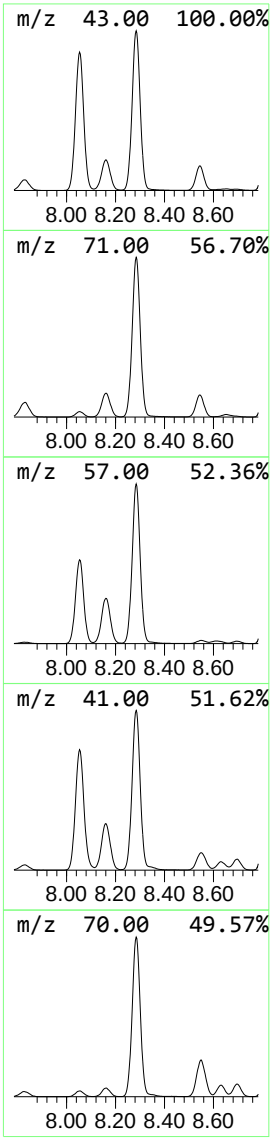
Peak Number 2 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	53.79 ug/l	18334300	Pentafluorobenzene	8.078

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	64
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	64
4	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	64
5	Heptane, 4-methyl-	114	C8H18	000589-53-7	64





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Instrument :
MSVOA_N
ClientSampleId :
41172

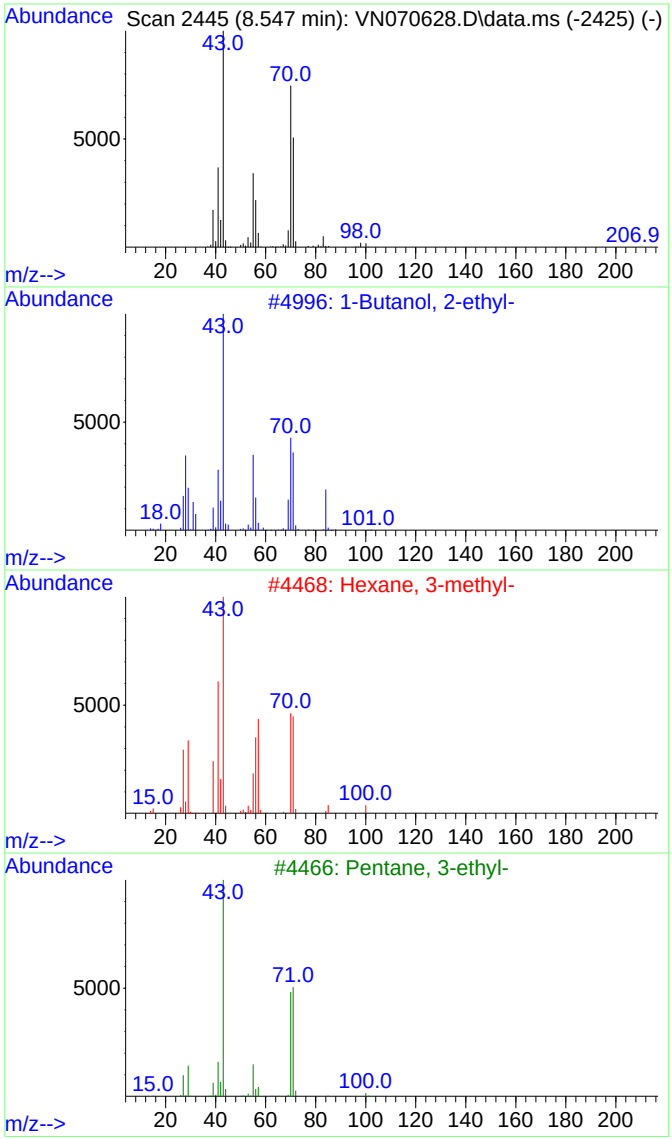
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

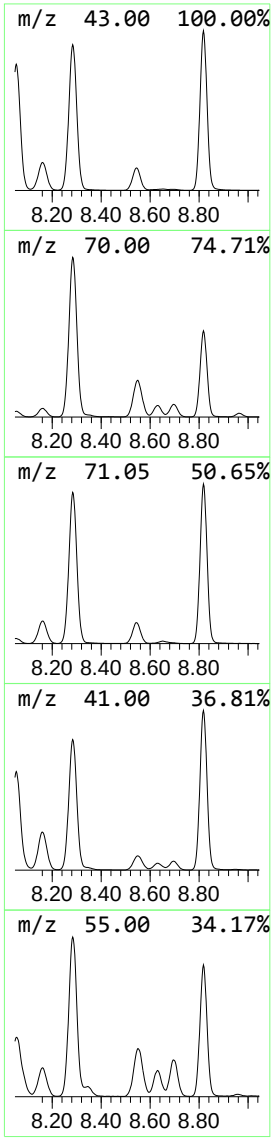
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Butanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.547	45.49 ug/l	2852390	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	47
4	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	47
5	1-Heptene, 4-methyl-	112	C8H16	013151-05-8	45





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Instrument :
MSVOA_N
ClientSampleId :
41172

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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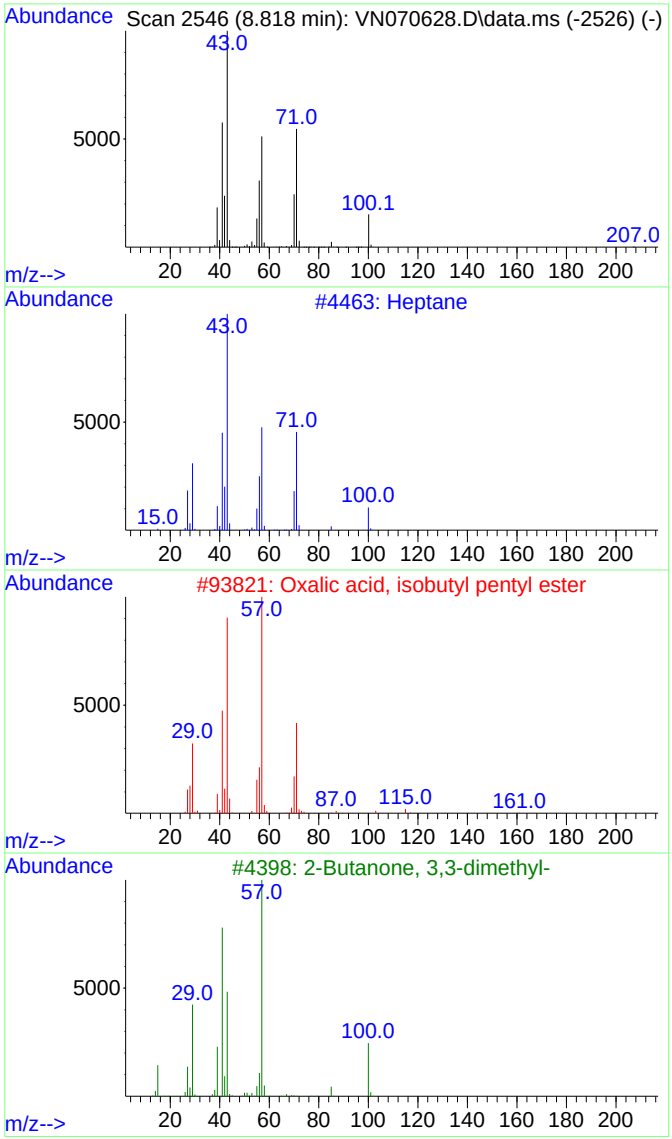
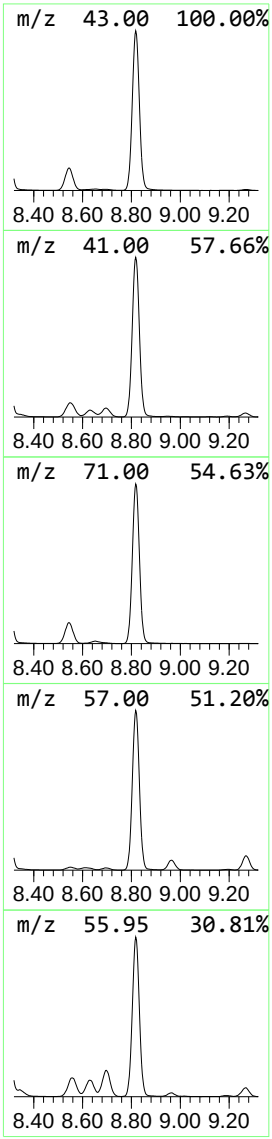
Peak Number 4 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.818	266.63 ug/l	16717500	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	95
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	43
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	42
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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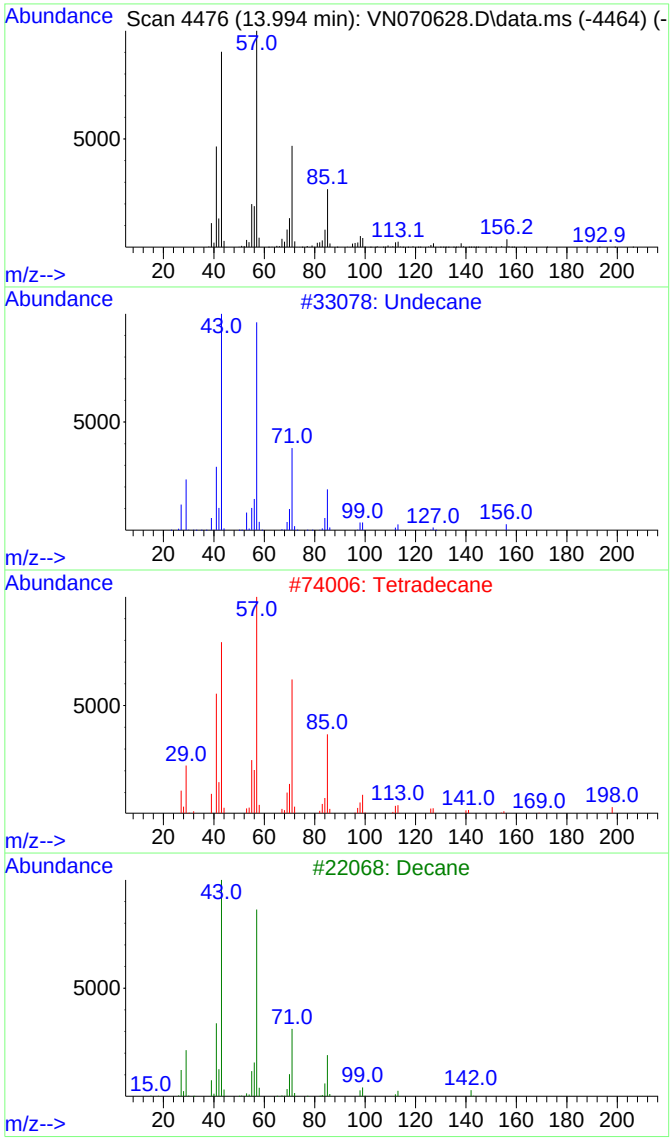
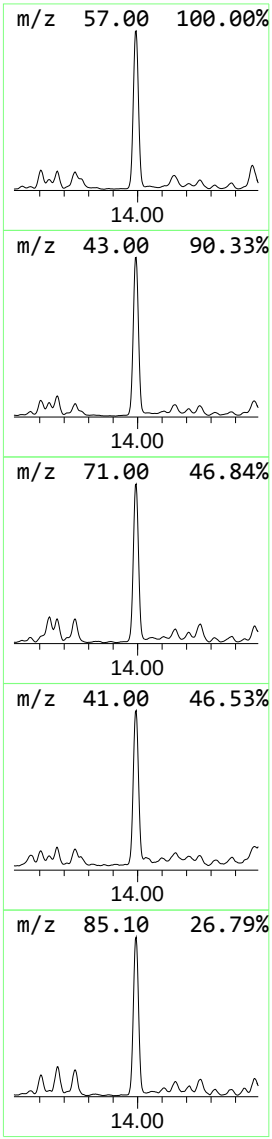
Peak Number 5 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	64.43 ug/l	4615290	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Tetradecane	198	C14H30	000629-59-4	90
3	Decane	142	C10H22	000124-18-5	90
4	Tridecane	184	C13H28	000629-50-5	86
5	Hexadecane	226	C16H34	000544-76-3	80





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MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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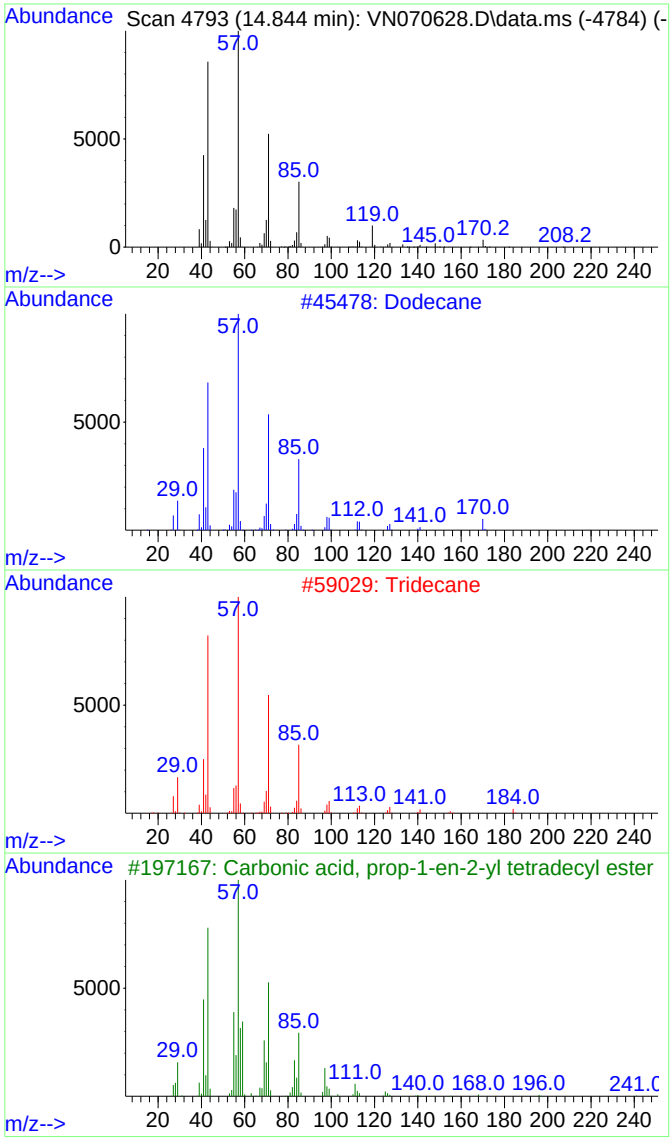
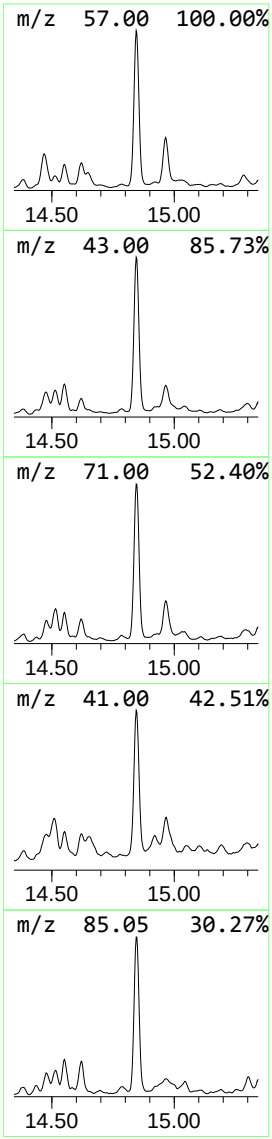
Peak Number 6 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.844	42.41 ug/l	3037750	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	95
2	Tridecane	184	C13H28	000629-50-5	80
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	80
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	80
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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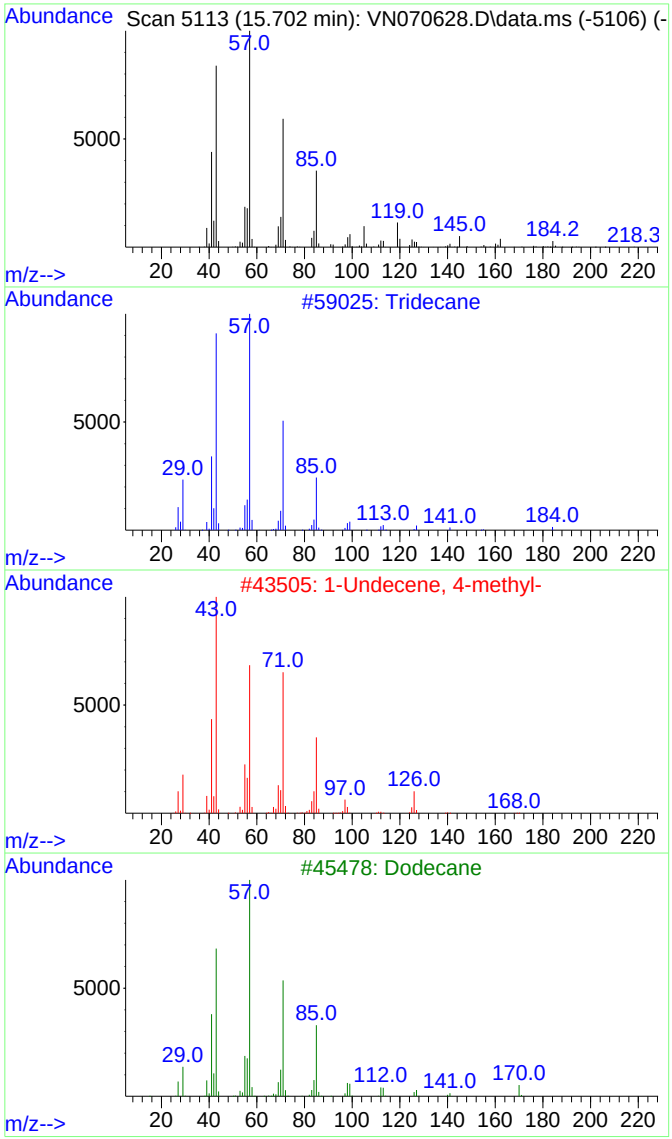
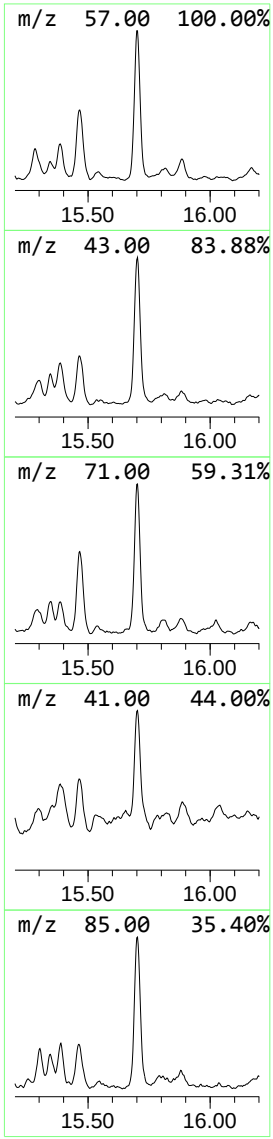
Peak Number 7 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.702	22.04 ug/l	1578750	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	1-Undecene, 4-methyl-	168	C12H24	074630-39-0	53
3	Dodecane	170	C12H26	000112-40-3	52
4	Tetradecane	198	C14H30	000629-59-4	52
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	52





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2,3-di...	8.161	13.9	ug/l	4719830	1	8.078	17041000	50.0
Hexane, 3-methyl-	8.284	53.8	ug/l	18334300	1	8.078	17041000	50.0
1-Butanol, 2-et...	8.547	45.5	ug/l	2852390	2	8.963	3134960	50.0
Heptane	8.818	266.6	ug/l	16717500	2	8.963	3134960	50.0
Undecane	13.994	64.4	ug/l	4615290	4	13.675	3581360	50.0
Dodecane	14.844	42.4	ug/l	3037750	4	13.675	3581360	50.0
Tridecane	15.702	22.0	ug/l	1578750	4	13.675	3581360	50.0