LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070362.D
Acq On : 29 Dec 2021 20:57
Operator : JC/MD
Sample : M5092-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

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: VN070362.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.856	317	323	334	rVB	63802	88087	1.32%	0.156%
2	4.307	843	864	901	rBV	81852	291377	4.38%	0.517%
3	4.854	1048	1068	1091	rBV	76363	244627	3.67%	0.434%
4	5.304	1213	1236	1258	rBV2	36304	135850	2.04%	0.241%
5	6.074	1504	1523	1548	rVB6	26732	89538	1.34%	0.159%
6	7.356	1978	2001	2029	rBV2	107659	376145	5.65%	0.667%
7	8.018	2222	2248	2259	rBV	742951	1829794	27.48%	3.246%
8	8.080	2259	2271	2301	rVB	1220387	2847729	42.77%	5.052%
9	8.434	2381	2403	2429	rBV	855438	2001990	30.07%	3.551%
10	8.686	2471	2497	2527	rBV5	116349	541971	8.14%	0.961%
11	8.850	2541	2558	2581	rVB4	65158	202512	3.04%	0.359%
12	8.965	2581	2601	2624	rBV	2120347	4469444	67.12%	7.928%
13	9.553	2799	2820	2842	rBV3	62479	177981	2.67%	0.316%
14	10.440	3133	3151	3165	rBV	3466443	6452277	96.90%	11.446%
15	10.505	3165	3175	3202	rVB	808524	1532634	23.02%	2.719%
16	11.092	3382	3394	3407	rBV2	33681	68609	1.03%	0.122%
17	11.194	3417	3432	3457	rVB	280990	535708	8.05%	0.950%
18	11.620	3571	3591	3607	rBV	237618	411842	6.18%	0.731%
19	11.746	3620	3638	3666	rBV	3664847	6658865	100.00%	11.812%
20	12.049	3738	3751	3763	rBV2	178131	302311	4.54%	0.536%
21	12.457	3890	3903	3916	rBV3	198583	373660	5.61%	0.663%
22	12.637	3959	3970	3984	rVB6	86425	155380	2.33%	0.276%
23	12.733	3989	4006	4030	rVV	3180479	5527937	83.02%	9.806%
24	12.841	4031	4046	4071	rVV2	563818	1216599	18.27%	2.158%
25	13.053	4115	4125	4136	rBV6	53411	95551	1.43%	0.169%
26	13.141	4149	4158	4170	rVB3	74962	123115	1.85%	0.218%
27	13.205	4171	4182	4197	rVB3	184615	305510	4.59%	0.542%
28	13.374	4234	4245	4246	rBV2	98861	112715	1.69%	0.200%
29	13.516	4280	4298	4311	rBV6	126104	276229	4.15%	0.490%
30	13.586	4311	4324	4331	rBV2	370392	645670	9.70%	1.145%
31	13.675	4343	4357	4371	rBV	3846091	6484325	97.38%	11.503%
32	13.739	4371	4381	4403	rVB2	595297	1053833	15.83%	1.869%
33	13.833	4405	4416	4431	rVB	120555	190648	2.86%	0.338%
34	14.198	4544	4552	4564	rVB	49723	82561	1.24%	0.146%
35	14.343	4587	4606	4632	rBV7	501376	1543737	23.18%	2.738%
36	14.447	4636	4645	4659	rVB2	127974	210708	3.16%	0.374%

LSC Area Percent Report

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

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

37	14.847	4785	4794	4809	rBV	137929	202768	3.05%	0.360%
38	14.970	4831	4840	4855	rVB5	167185	331685	4.98%	0.588%
39	15.102	4881	4889	4896	rBV8	90981	148279	2.23%	0.263%
40	15.469	5017	5026	5040	rBV5	393436	690261	10.37%	1.224%
41	15.700	5103	5112	5131	rVB	990898	1699443	25.52%	3.015%
42	16.268	5314	5324	5346	rBV8	820270	2010624	30.19%	3.567%
43	16.464	5388	5397	5415	rVB3	805489	1644863	24.70%	2.918%
44	16.679	5467	5477	5490	rVB2	1112801	1986880	29.84%	3.525%

Sum of corrected areas: 56372272

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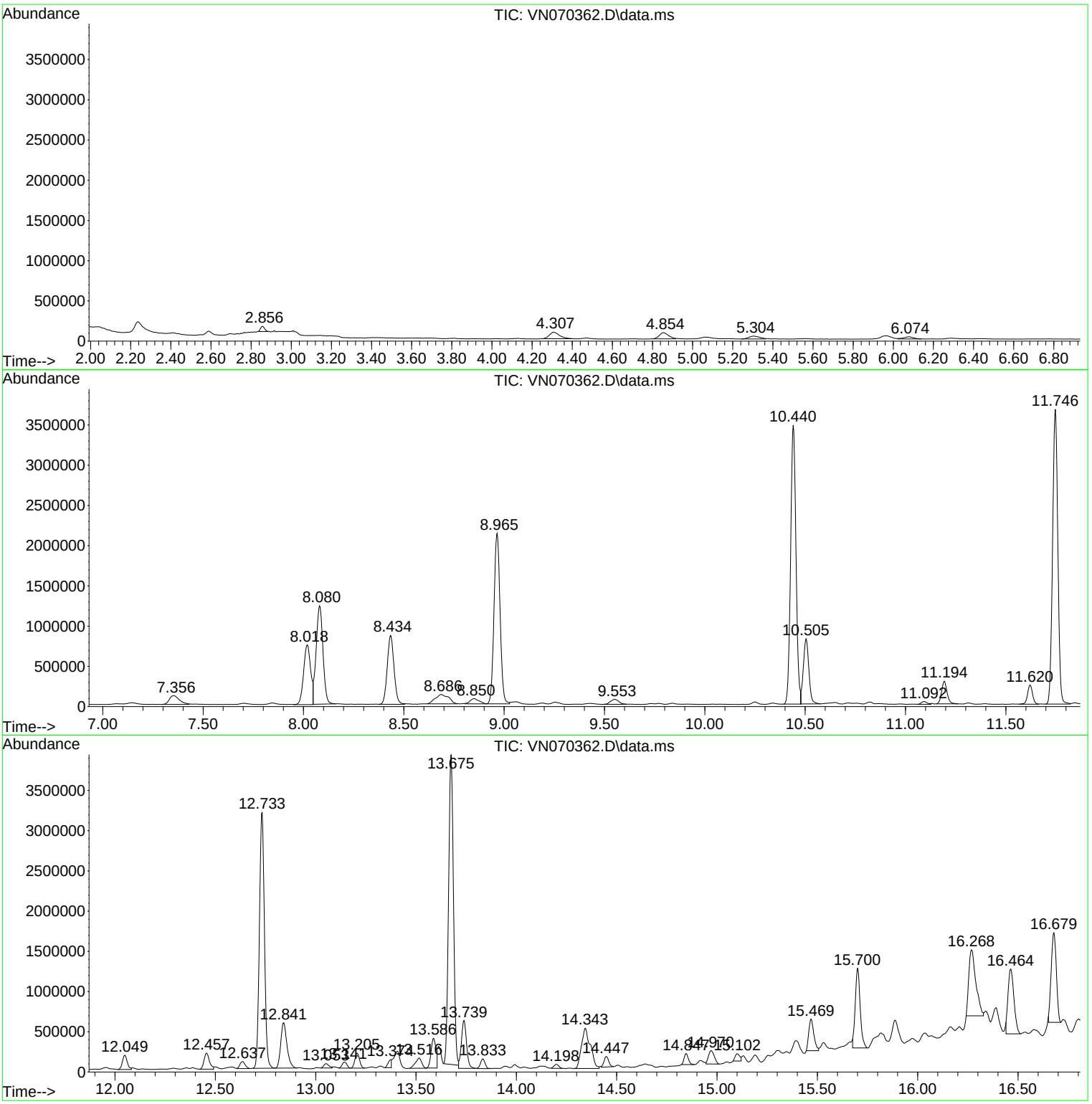
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070362.D
Acq On : 29 Dec 2021 20:57
Operator : JC/MD
Sample : M5092-05
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

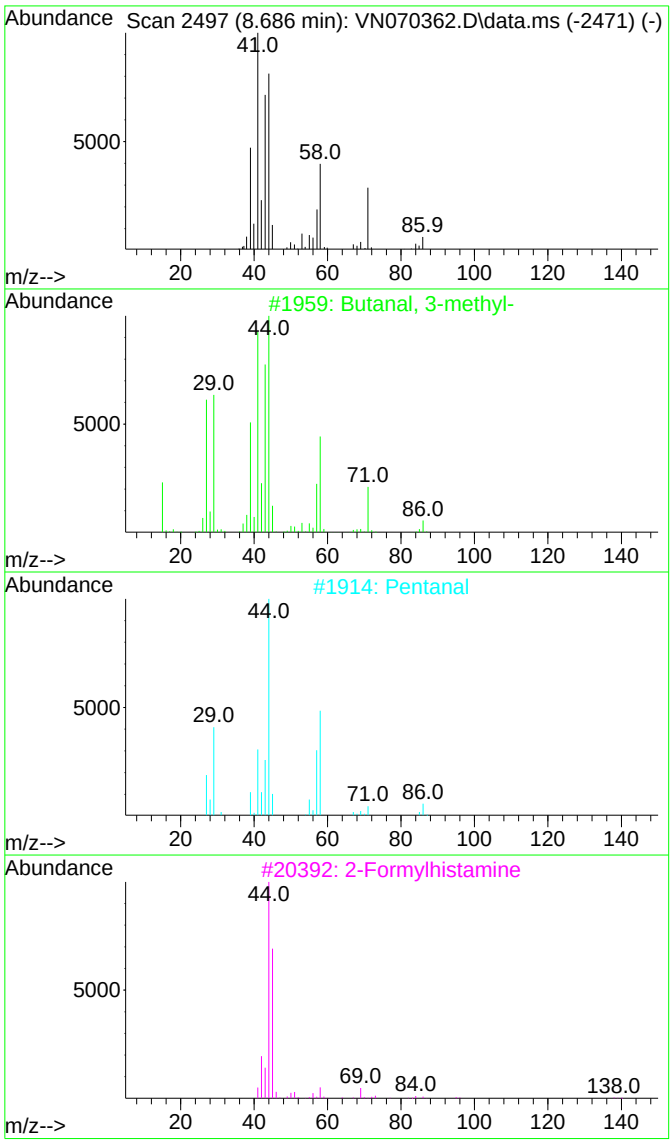
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

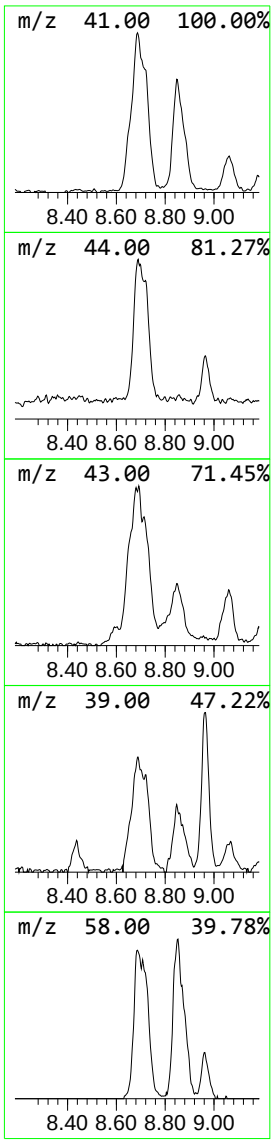
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butanal, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.686	6.06 ug/l	541971	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 3-methyl-	86	C5H10O	000590-86-3	94
2	Pentanal	86	C5H10O	000110-62-3	49
3	2-Formylhistamine	139	C6H9N3O	1000132-95-8	23
4	3,3-Dimethyl-4-methylamino-butan...	129	C7H15NO	123528-99-4	12
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	10





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Operator : JC/MD
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Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

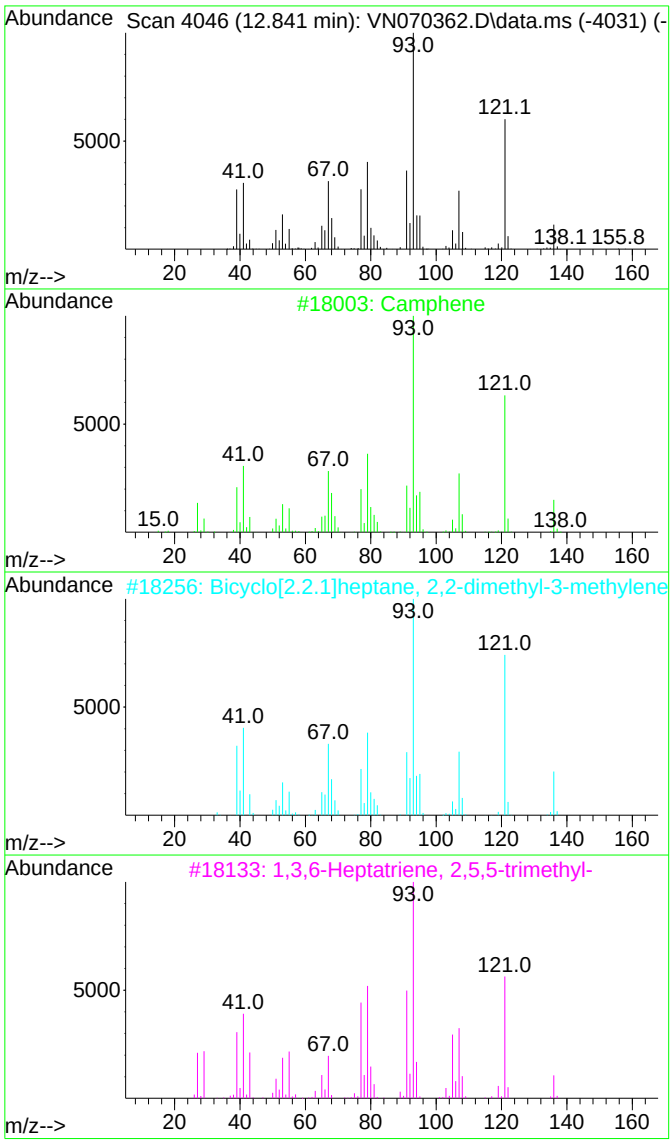
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

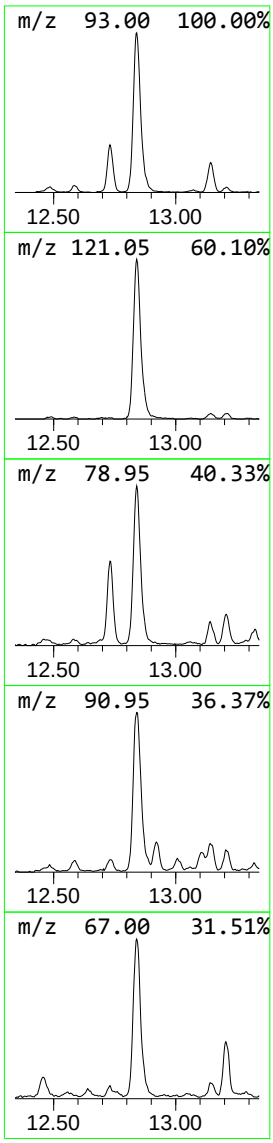
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Camphene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	9.38 ug/l	1216600	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	97
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	95
3	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	91
4	(+)-4-Carene	136	C10H16	029050-33-7	87
5	Cyclohexene, 1-methyl-3-(1-methy...	136	C10H16	000499-03-6	86





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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

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

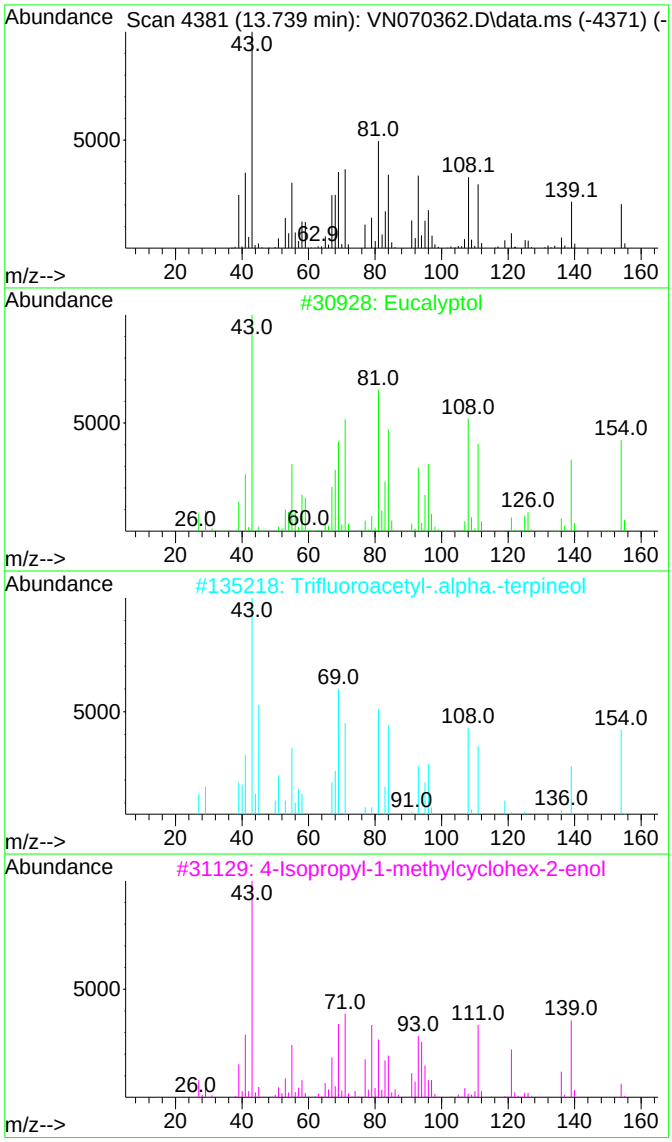
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

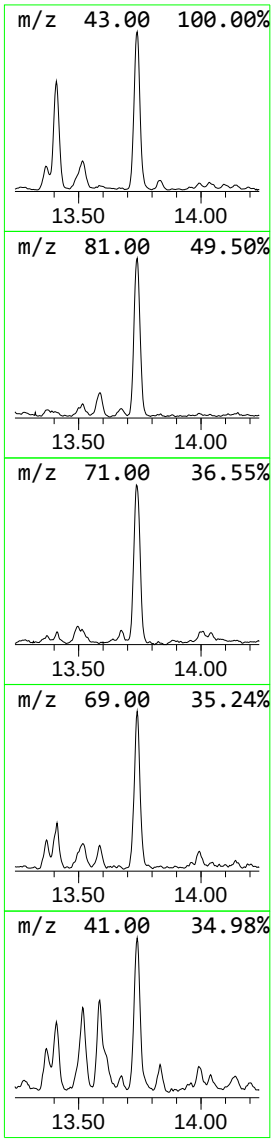
****

Peak Number 3 Eucalyptol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	8.13 ug/l	1053830	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	43
4	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	38
5	1-Cyclopentene-1-methanol, .alph...	154	C10H18O	056666-69-4	27





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Sample : M5092-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

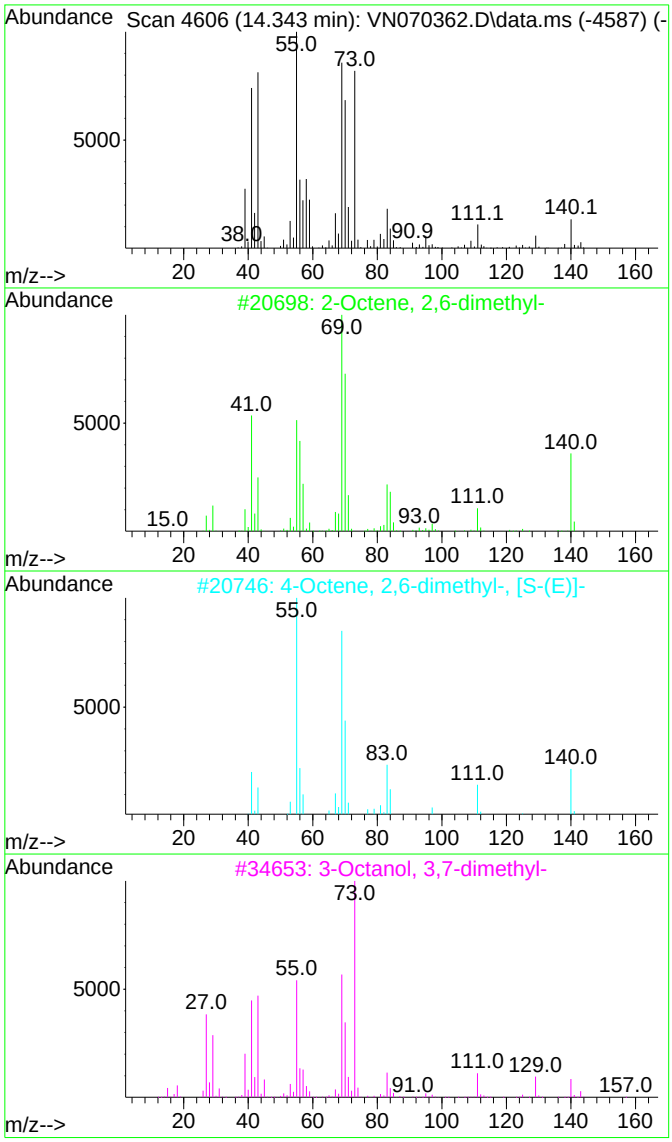
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

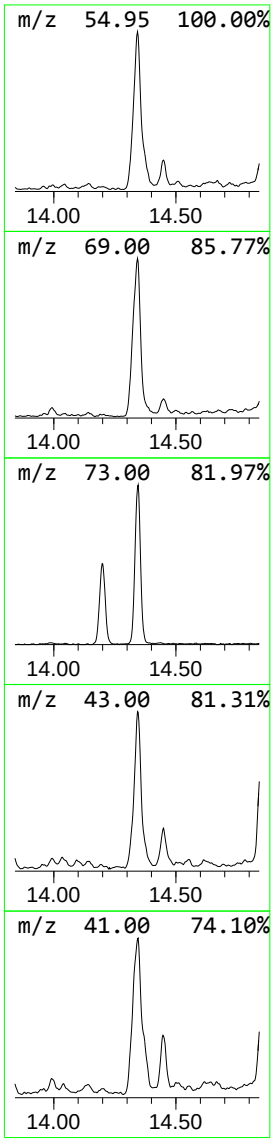
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Octene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.342	11.90 ug/l	1543740	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	58
2	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	55
3	3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	53
4	3-Nonene, 3-methyl-, (E)-	140	C10H20	069405-42-1	52
5	3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	49





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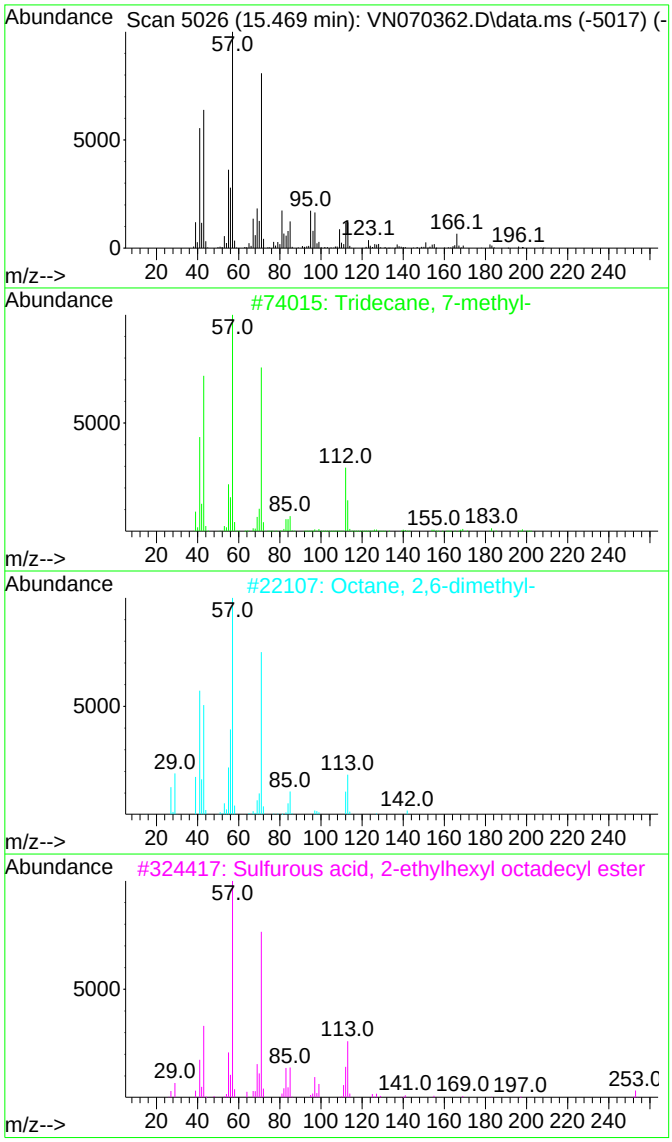
Quant Title : SW846 8260

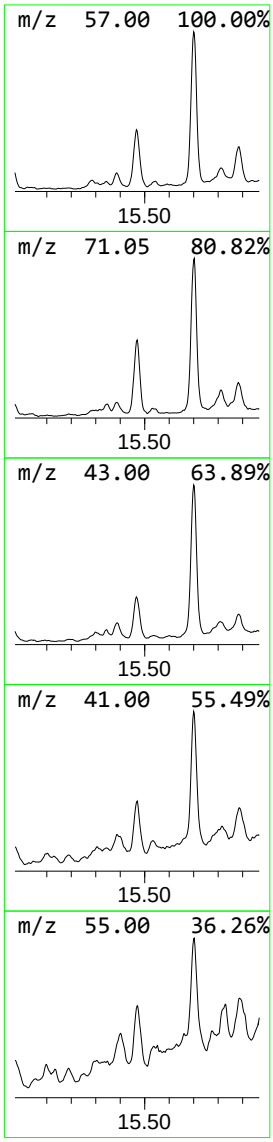
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Tridecane, 7-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	5.32 ug/l	690261	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 7-methyl-	198	C14H30	026730-14-3	86
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	80
3	Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	64
4	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
5	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	59





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Quant Title : SW846 8260

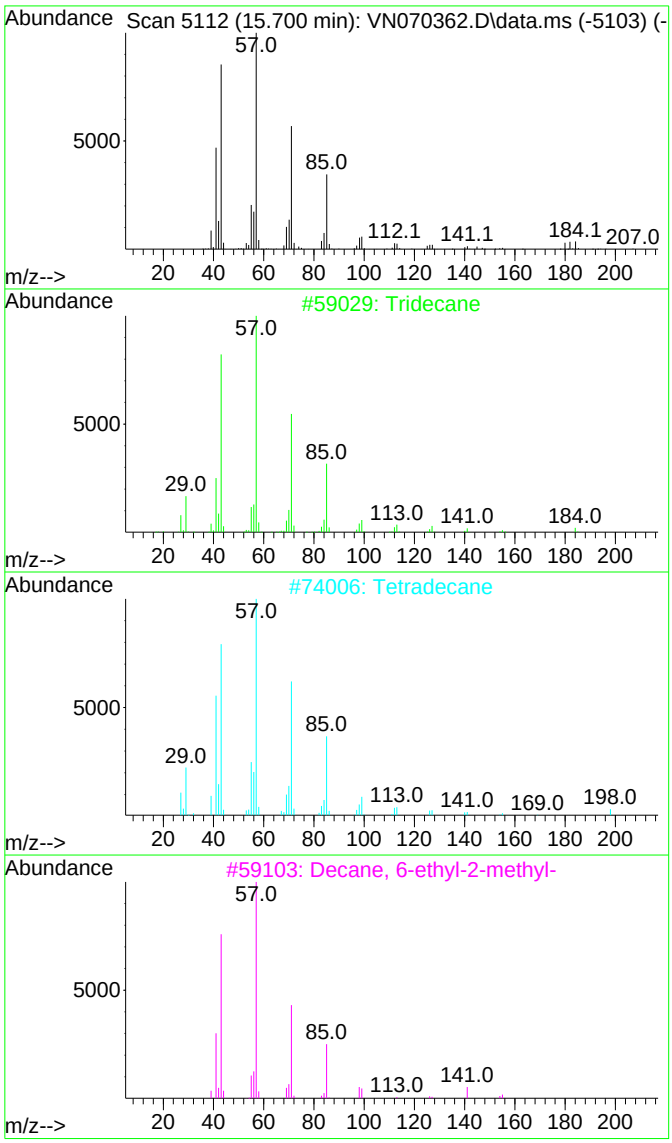
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

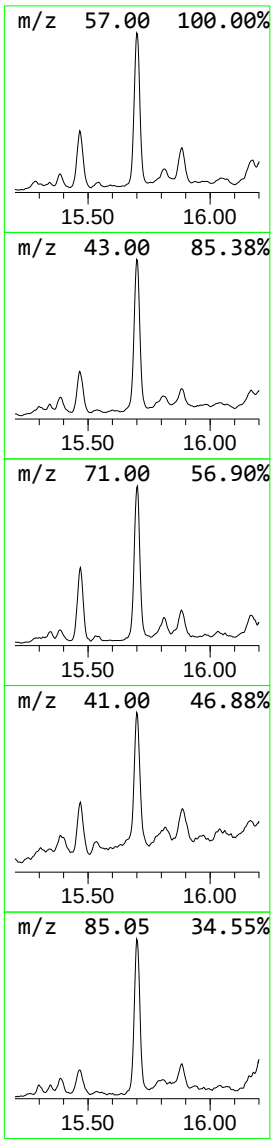
****

Peak Number 6 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.700	13.10 ug/l	1699440	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Tetradecane	198	C14H30	000629-59-4	86
3	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78
4	Hexadecane	226	C16H34	000544-76-3	72
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	64





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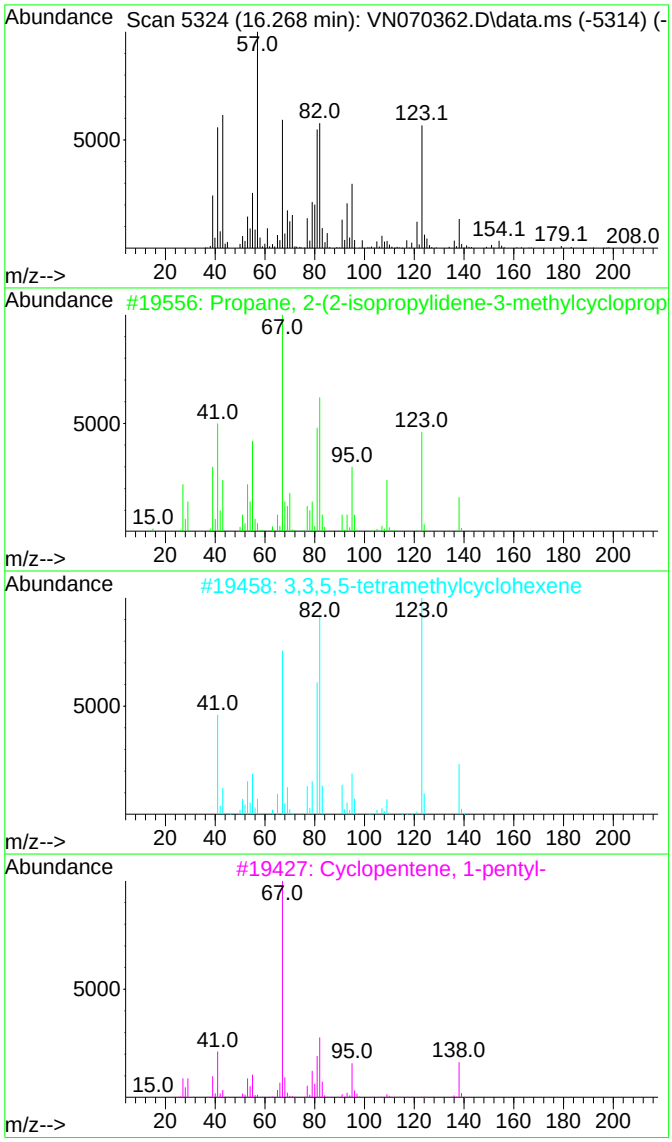
Quant Title : SW846 8260

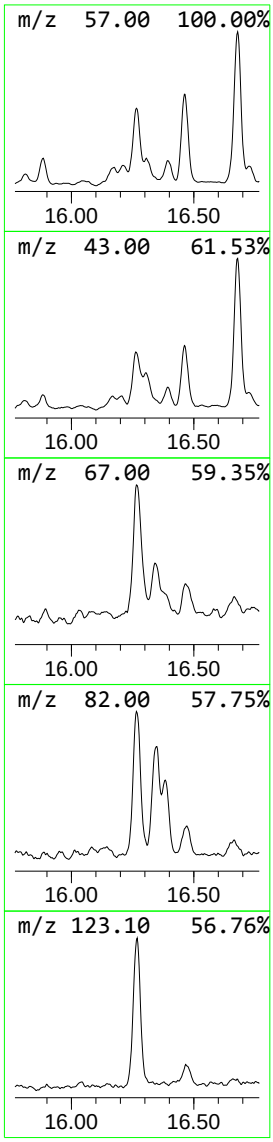
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propane, 2-(2-isopropyliden... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.268	15.50 ug/l	2010620	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-(2-isopropylidene-3-m...	138	C10H18	024524-51-4	62
2	3,3,5,5-tetramethylcyclohexene	138	C10H18	1000510-60-7	53
3	Cyclopentene, 1-pentyl-	138	C10H18	004291-98-9	46
4	Phenol, 4-methoxy-3-methyl-	138	C8H10O2	014786-82-4	46
5	trans-Chrysanthemol	154	C10H18O	018383-58-9	42





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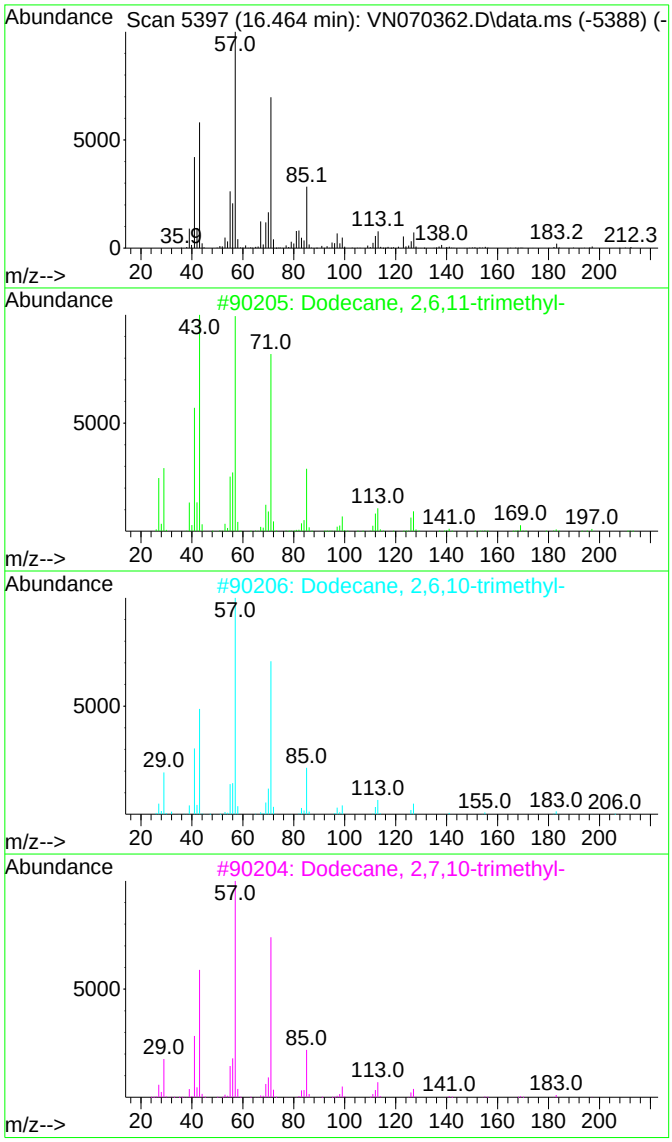
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

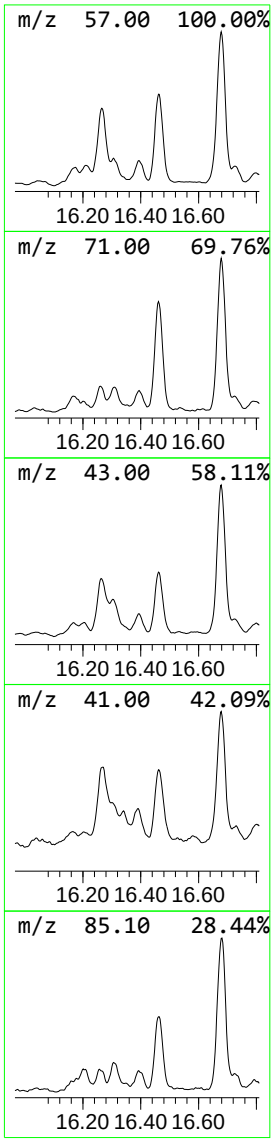
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.464	12.68 ug/l	1644860	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	93
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	91
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	87
4	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	81
5	Decane, 5-propyl-	184	C13H28	017312-62-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070362.D
Acq On : 29 Dec 2021 20:57
Operator : JC/MD
Sample : M5092-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

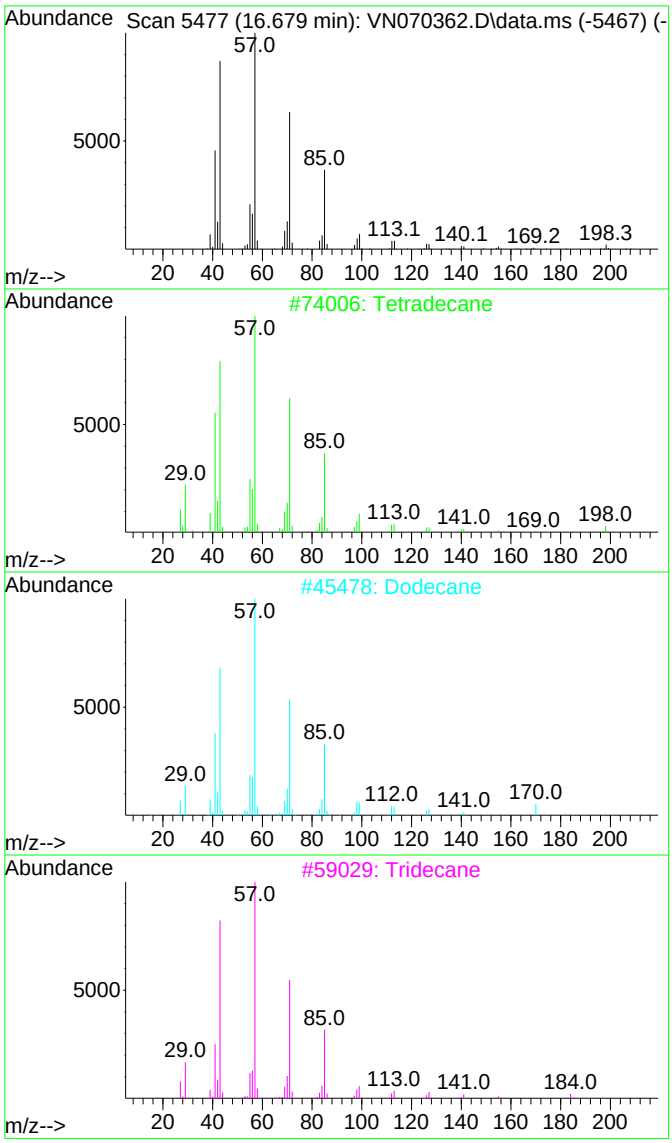
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

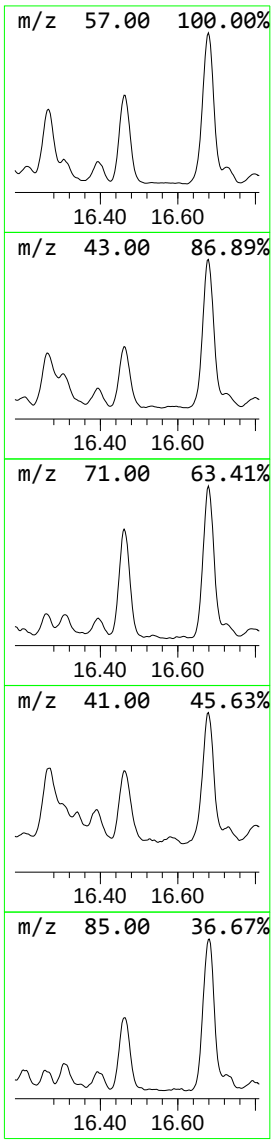
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.679	15.32 ug/l	1986880	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	97
2	Dodecane	170	C12H26	000112-40-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070362.D
Acq On : 29 Dec 2021 20:57
Operator : JC/MD
Sample : M5092-05
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PATAPSCO-FEED-PELLETS

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal, 3-methyl-	8.686	6.1	ug/l	541971	2	8.965	4469440	50.0
Camphene	12.841	9.4	ug/l	1216600	4	13.675	6484330	50.0
Eucalyptol	13.739	8.1	ug/l	1053830	4	13.675	6484330	50.0
2-Octene, 2,6-d...	14.342	11.9	ug/l	1543740	4	13.675	6484330	50.0
Tridecane, 7-me...	15.469	5.3	ug/l	690261	4	13.675	6484330	50.0
Tridecane	15.700	13.1	ug/l	1699440	4	13.675	6484330	50.0
Propane, 2-(2-i...	16.268	15.5	ug/l	2010620	4	13.675	6484330	50.0
Dodecane, 2,6,1...	16.464	12.7	ug/l	1644860	4	13.675	6484330	50.0
Tetradecane	16.679	15.3	ug/l	1986880	4	13.675	6484330	50.0