LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036949.D
Acq On : 11 Aug 2023 18:27
Operator : JC/MD
Sample : 03961-03ME 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071ME

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_X\Method\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.563	69	78	80	rBV4	3599	8892	1.27%	0.161%
2	4.593	564	575	591	rBV2	5944	21494	3.06%	0.390%
3	5.385	693	705	720	rBV2	79894	233678	33.31%	4.238%
4	5.550	720	732	747	rVB	130176	367537	52.39%	6.666%
5	5.958	789	799	816	rBV	85613	224498	32.00%	4.071%
6	6.763	921	931	946	rBV	214041	508452	72.48%	9.221%
7	8.647	1229	1240	1251	rBV	442820	701546	100.00%	12.723%
8	10.055	1465	1471	1483	rVB	478381	638167	90.97%	11.574%
9	10.299	1507	1511	1518	rVB	8445	12533	1.79%	0.227%
10	11.079	1634	1639	1652	rBV	389905	502463	71.62%	9.113%
11	11.378	1683	1688	1690	rBV	9932	12026	1.71%	0.218%
12	11.750	1745	1749	1755	rBV	22749	28698	4.09%	0.520%
13	12.024	1788	1794	1800	rBV	486164	625375	89.14%	11.342%
14	12.317	1838	1842	1851	rVB4	6989	13302	1.90%	0.241%
15	12.817	1918	1924	1928	rBV3	8419	13072	1.86%	0.237%
16	12.920	1932	1941	1945	rBV3	9820	16502	2.35%	0.299%
17	13.164	1975	1981	1986	rBV7	3577	7811	1.11%	0.142%
18	13.292	1998	2002	2007	rVB3	11802	16025	2.28%	0.291%
19	13.408	2016	2021	2028	rBV7	11635	26612	3.79%	0.483%
20	13.469	2028	2031	2034	rVB	5879	7616	1.09%	0.138%
21	13.518	2034	2039	2042	rBV4	7111	13160	1.88%	0.239%
22	13.585	2047	2050	2054	rBV4	4481	7390	1.05%	0.134%
23	13.676	2061	2065	2070	rBV8	8016	15575	2.22%	0.282%
24	13.768	2077	2080	2083	rBV2	11696	14652	2.09%	0.266%
25	13.798	2083	2085	2088	rVB3	15284	16131	2.30%	0.293%
26	13.847	2089	2093	2100	rBV6	23454	38925	5.55%	0.706%
27	13.914	2100	2104	2105	rBV3	8883	12351	1.76%	0.224%
28	14.066	2125	2129	2132	rBV4	26277	36640	5.22%	0.665%
29	14.164	2143	2145	2150	rVB4	11862	18350	2.62%	0.333%
30	14.219	2150	2154	2158	rBV4	26060	43023	6.13%	0.780%
31	14.481	2194	2197	2205	rBV5	26299	65510	9.34%	1.188%
32	14.548	2206	2208	2209	rBV2	14610	12488	1.78%	0.226%
33	14.615	2216	2219	2225	rBV4	83158	141531	20.17%	2.567%
34	14.670	2225	2228	2232	rBV3	43750	59057	8.42%	1.071%
35	14.749	2239	2241	2244	rBV3	36418	45533	6.49%	0.826%
36	14.786	2244	2247	2250	rVV3	38434	51629	7.36%	0.936%

LSC Area Percent Report

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071ME

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_X\Method\82X072123W.M
Title : SW846 8260

37	14.847	2254	2257	2261	rVB3	48718	59832	8.53%	1.085%
38	15.176	2307	2311	2314	rBV4	65440	110317	15.72%	2.001%
39	15.377	2341	2344	2346	rVB3	36178	38980	5.56%	0.707%
40	15.414	2346	2350	2355	rVB2	97753	139513	19.89%	2.530%
41	15.481	2358	2361	2365	rBV3	50257	83876	11.96%	1.521%
42	15.609	2380	2382	2386	rVB	46608	53997	7.70%	0.979%
43	15.737	2398	2403	2409	rVB2	113677	226278	32.25%	4.104%
44	16.091	2457	2461	2472	rVB6	49423	110813	15.80%	2.010%
45	16.603	2542	2545	2556	rVB8	27898	68760	9.80%	1.247%
46	16.706	2557	2562	2571	rVV4	21711	43302	6.17%	0.785%

Sum of corrected areas: 5513912

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MSVOA_X
ClientSampleId :
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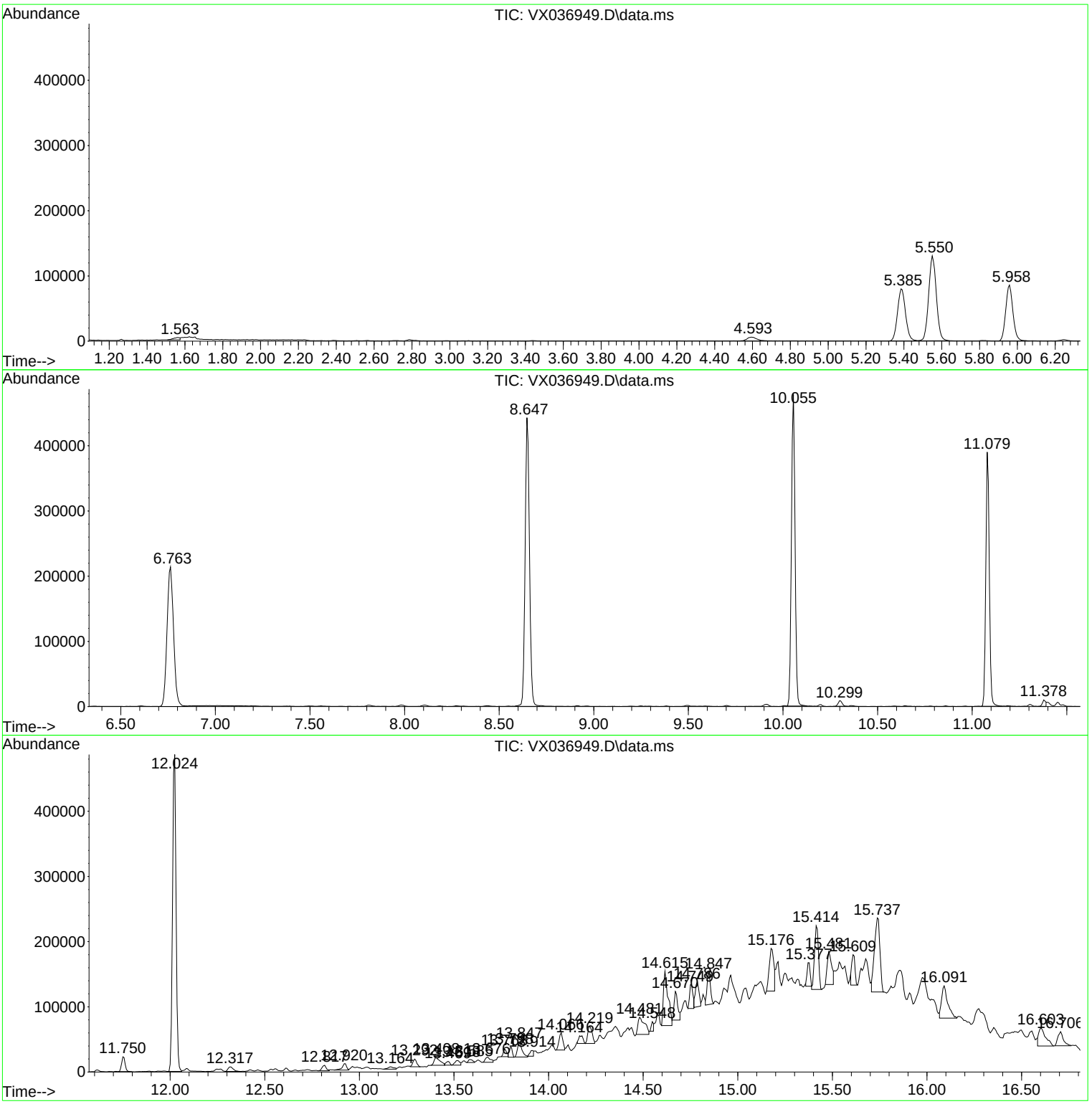
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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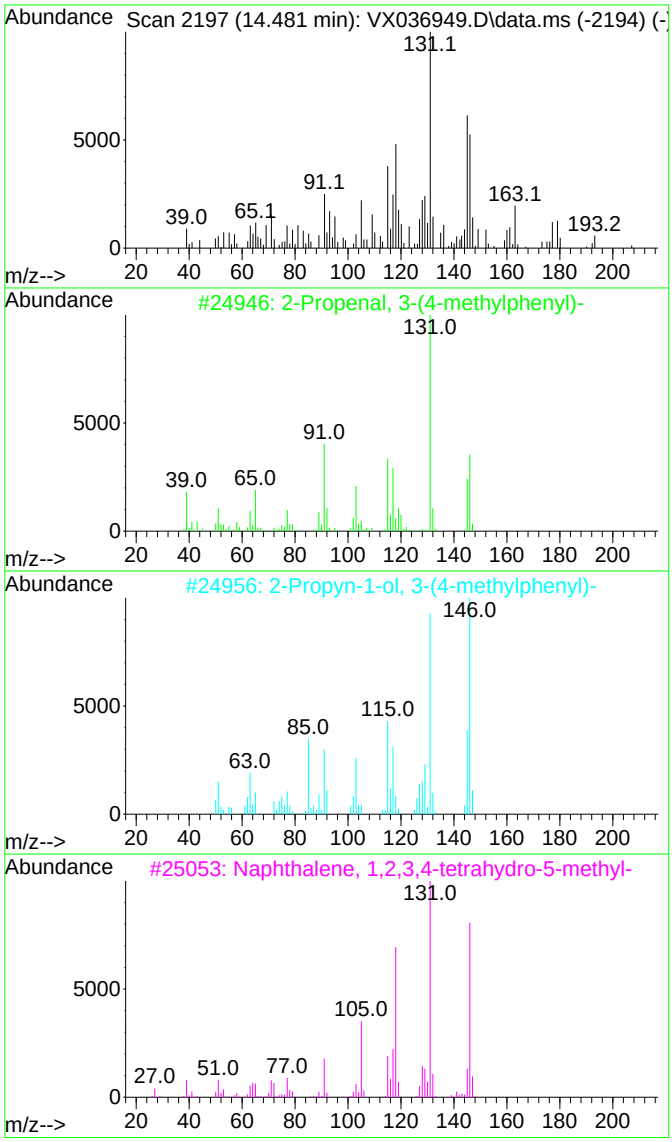
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

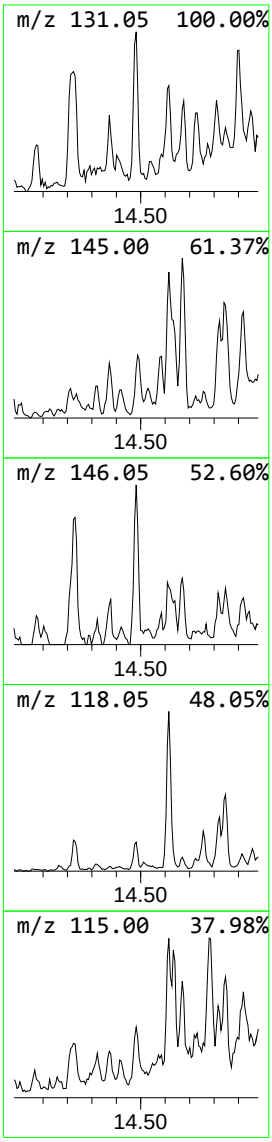
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propenal, 3-(4-methylphen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	5.24 ug/l	65510	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	55
2	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	53
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	52
4	2-(2-Hydroxyphenyl)buta-1,3-diene	146	C10H10O	038865-47-3	52
5	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	49





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Instrument :
MSVOA_X
ClientSampleId :
20071ME

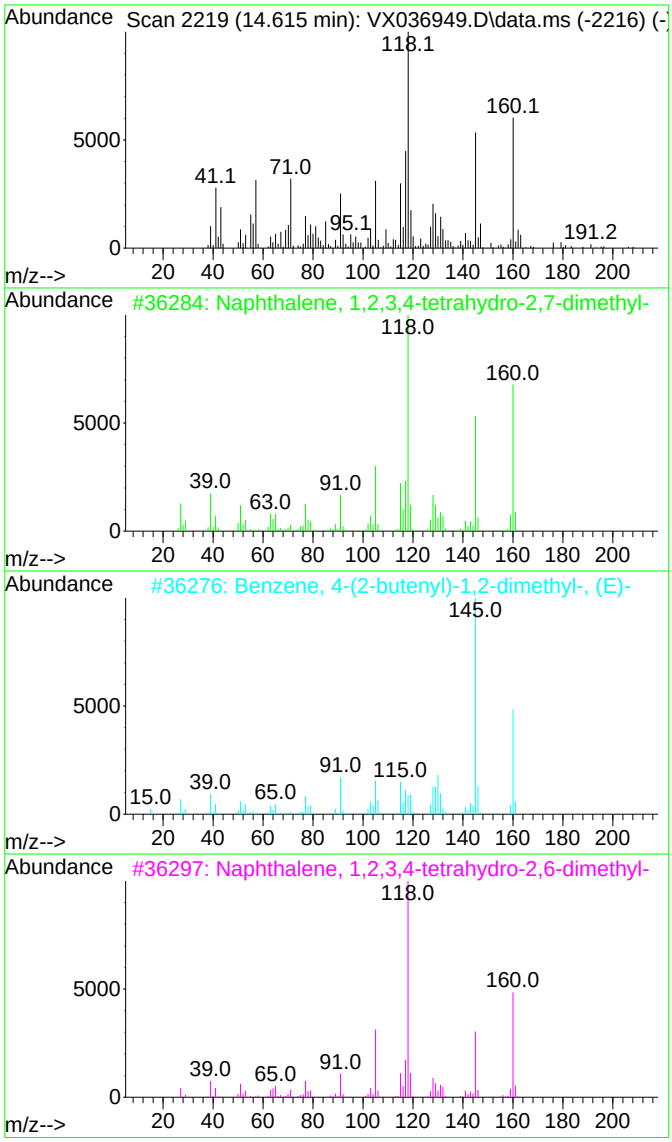
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

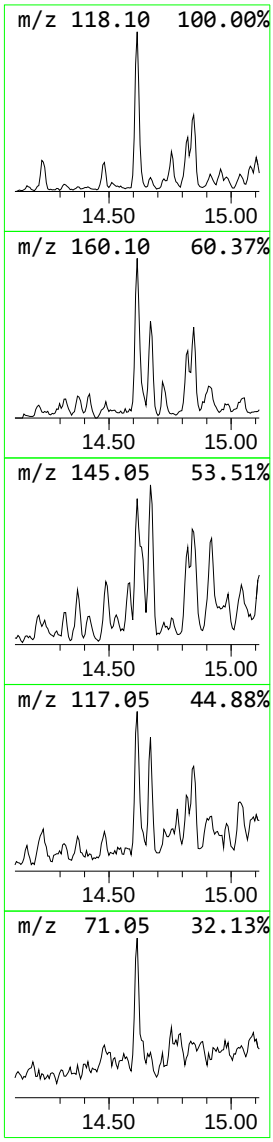
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	11.32 ug/l	141531	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	72
2	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	60
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	50
4	Diboroxide, trimethylphenyl-	160	C9H14B2O	1000162-60-0	49
5	Phenethyl alcohol, 2-(1-hydroxye...	180	C11H16O2	030314-65-9	43





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Sample : 03961-03ME 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071ME

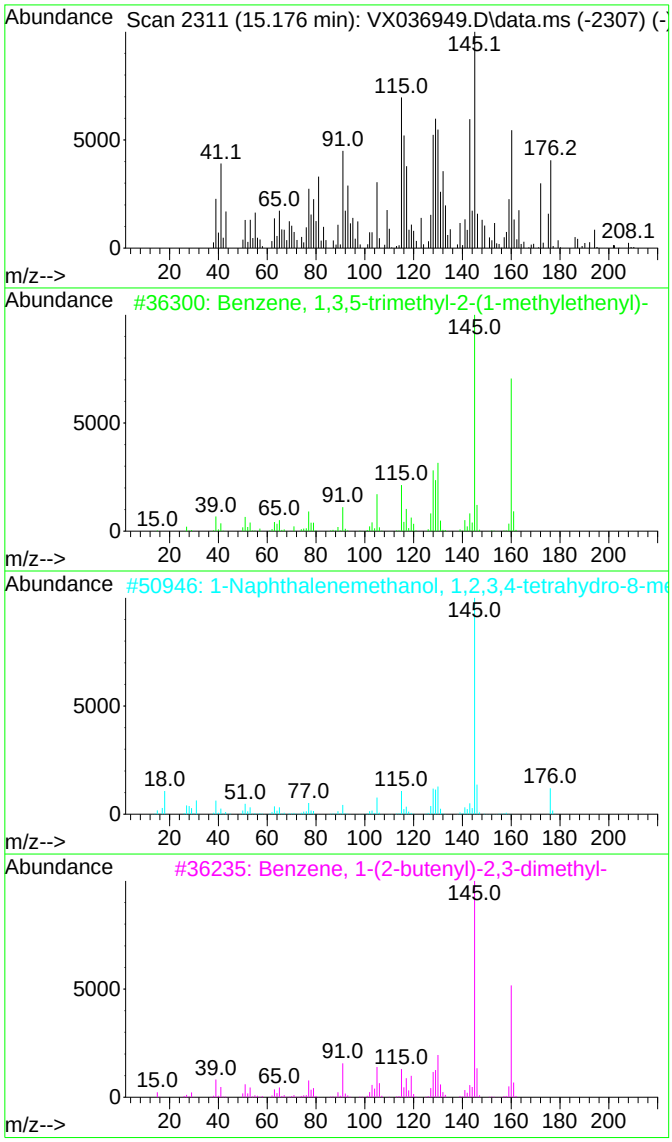
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

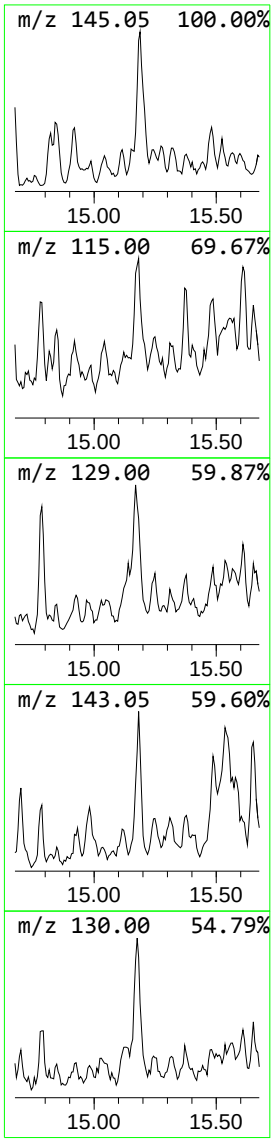
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.176	8.82 ug/l	110317	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	90
2	1-Naphthalenemethanol, 1,2,3,4-t...	176	C12H16O	036052-28-5	53
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	49
4	Oct-3-ene-1,5-diyne, 3-isopropyl...	160	C12H16	1000211-23-1	43
5	Methyl 3-(2-methylphenyl)prop-2-...	176	C11H12O2	075950-75-3	38





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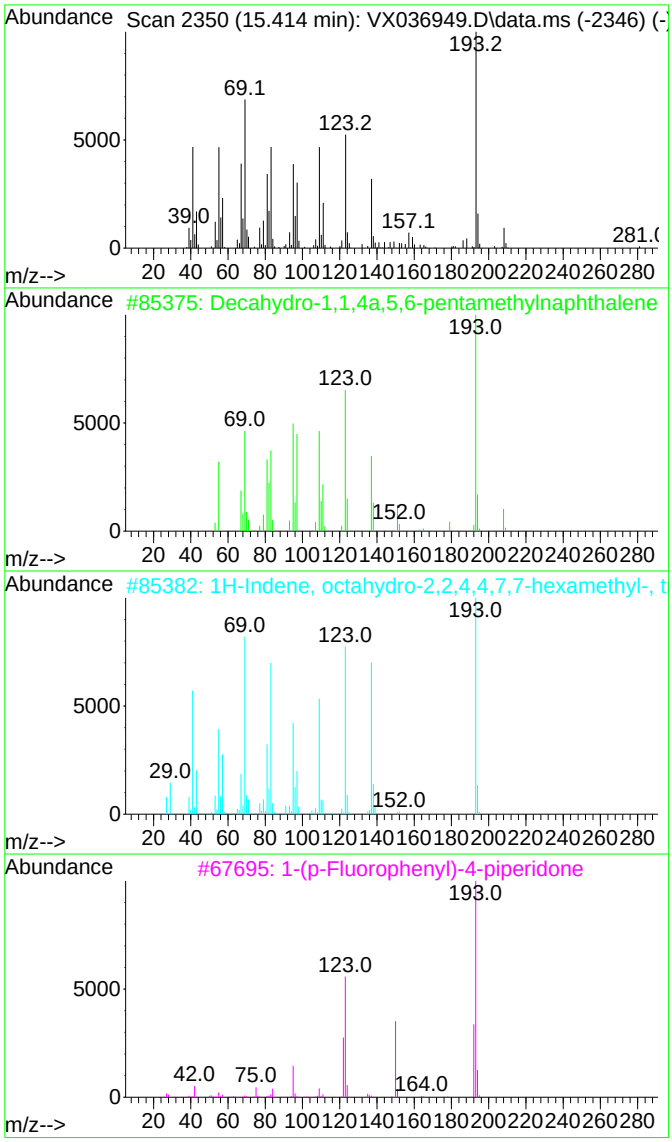
Quant Title : SW846 8260

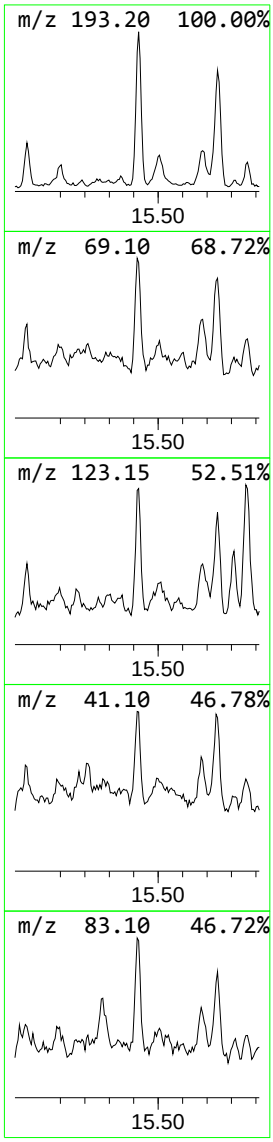
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	11.15 ug/l	139513	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	64
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4	Iminostilbene	193	C14H11N	000256-96-2	27
5	3-((2R,5S)-7-(Cyclohexylsulfonyl...	340	C17H28N2O3S	1000483-82-6	16





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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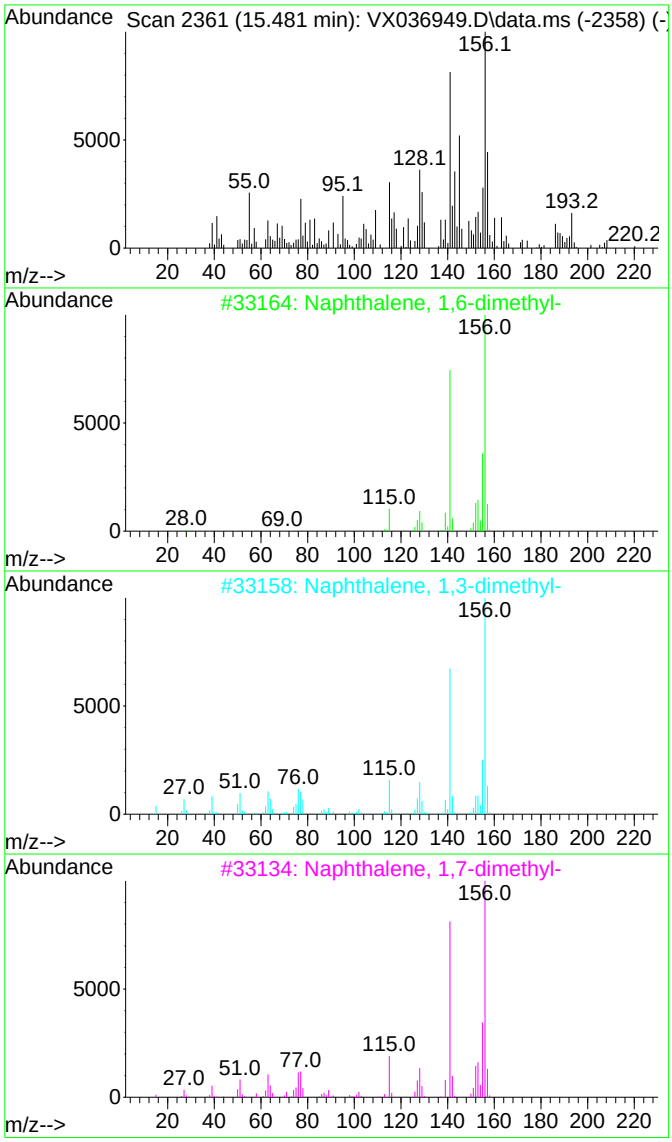
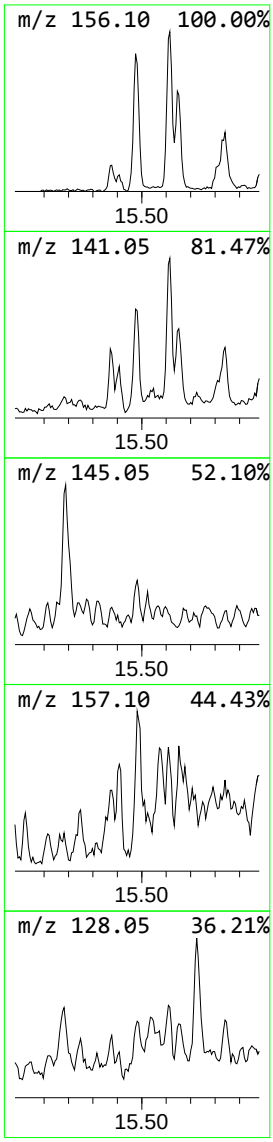
****
Peak Number 5 Naphthalene, 1,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	6.71 ug/l	83876	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	60
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	58
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	53
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	53
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	49





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Quant Title : SW846 8260

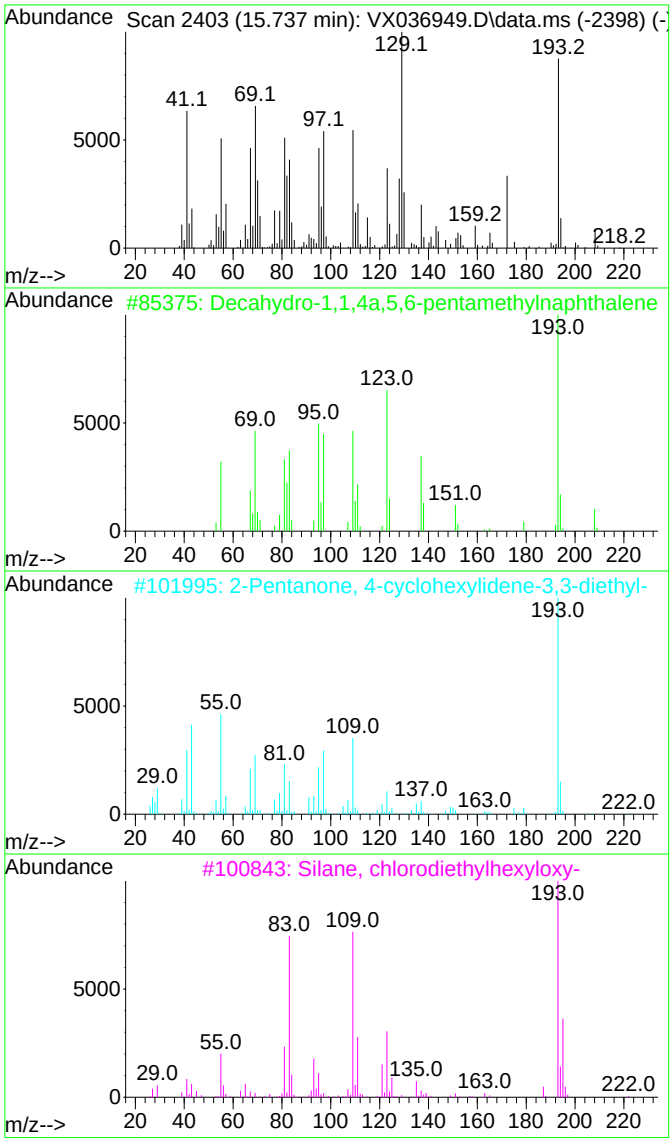
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

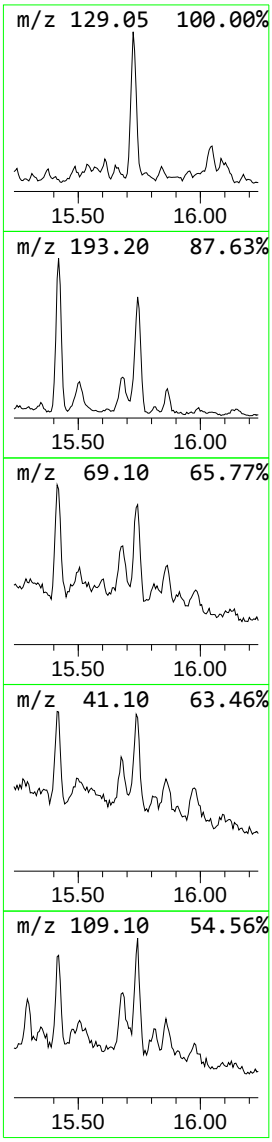
****

Peak Number 6 unknown15.737 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.737	18.09 ug/l	226278	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	87
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	22
4	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	14
5	1-Methyl-5-nitro-1H-benzoimidazo...	193	C8H7N3O3	066108-85-8	11





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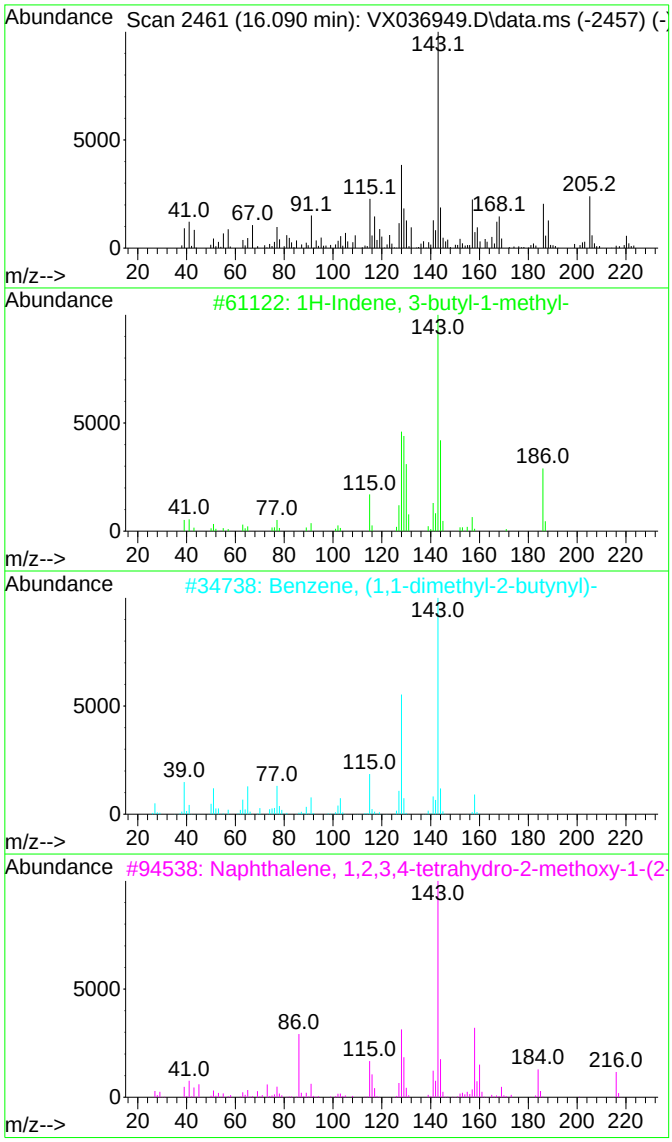
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

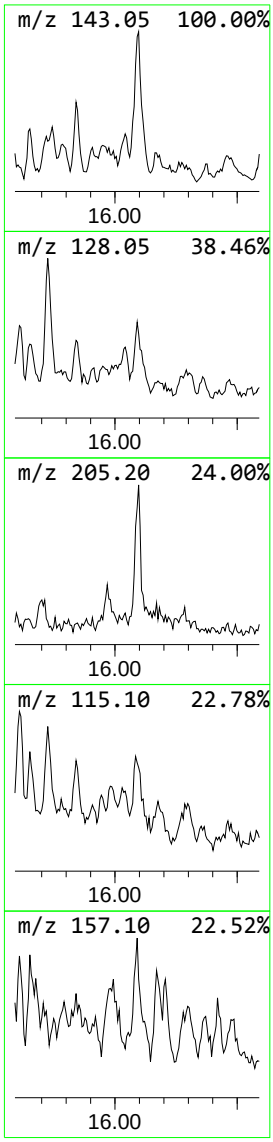
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 3-butyl-1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.090	8.86 ug/l	110813	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 3-butyl-1-methyl-	186	C14H18	111400-84-1	52
2	Benzene, (1,1-dimethyl-2-butynyl)-	158	C12H14	001007-91-6	46
3	Naphthalene, 1,2,3,4-tetrahydro-...	216	C15H20O	068156-99-0	43
4	1-(2-Methyl-propenyl)-1,2,3,4-te...	202	C14H18O	1370512-24-5	43
5	2-Methyl-1,2,3,4-tetrahydro-.bet...	186	C12H14N2	013100-00-0	38





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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

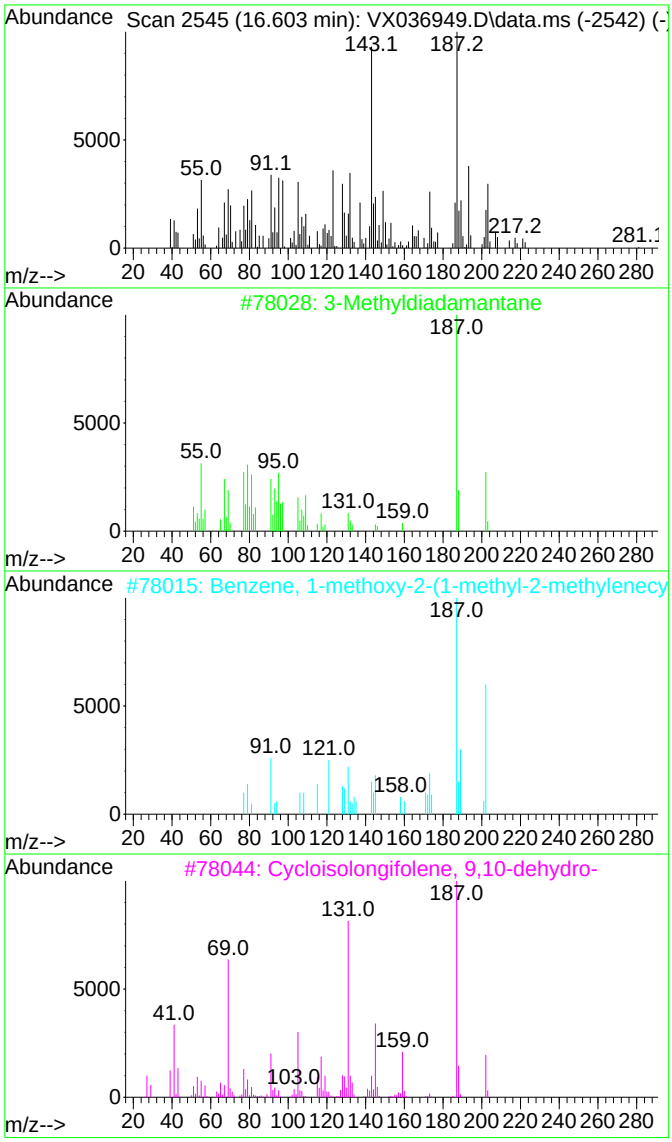
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

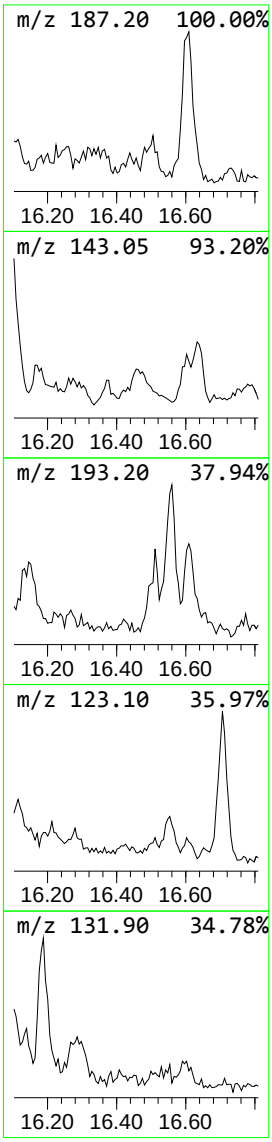
****

Peak Number 8 unknown16.603 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.603	5.50 ug/l	68760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyldiadamantane	202	C15H22	028375-86-2	35
2	Benzene, 1-methoxy-2-(1-methyl-2...	202	C14H18O	039877-94-6	35
3	Cycloisolongifolene, 9,10-dehydro-	202	C15H22	1000156-81-6	30
4	2-Chloro-6-fluorophenylacetic acid	188	C8H6ClFO2	037777-76-7	30
5	Pyrimidine-1-oxide, 2-amino-4-ph...	187	C10H9N3O	080830-43-9	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036949.D
Acq On : 11 Aug 2023 18:27
Operator : JC/MD
Sample : 03961-03ME 10X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
2-Propenal, 3-(...	14.481	5.2	ug/l	65510	4	12.024	625375	50.0
Naphthalene, 1,...	14.615	11.3	ug/l	141531	4	12.024	625375	50.0
Benzene, 1,3,5-...	15.176	8.8	ug/l	110317	4	12.024	625375	50.0
Decahydro-1,1,4...	15.414	11.2	ug/l	139513	4	12.024	625375	50.0
Naphthalene, 1,...	15.481	6.7	ug/l	83876	4	12.024	625375	50.0
unknown15.737	15.737	18.1	ug/l	226278	4	12.024	625375	50.0
1H-Indene, 3-bu...	16.090	8.9	ug/l	110813	4	12.024	625375	50.0
unknown16.603	16.603	5.5	ug/l	68760	4	12.024	625375	50.0