LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
Data File : VX034625.D
Acq On : 20 Mar 2023 14:11
Operator : JC/MD
Sample : 01939-04 20X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034625.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	79	rBV3	11726	22875	1.89%	0.241%
2	5.385	693	705	718	rBV2	136719	395928	32.74%	4.166%
3	5.550	721	732	746	rVB	235444	668438	55.28%	7.033%
4	5.952	787	798	815	rBV	185008	508385	42.04%	5.349%
5	6.757	920	930	945	rBV	422465	1034368	85.54%	10.883%
6	8.647	1233	1240	1251	rBV	762438	1209212	100.00%	12.723%
7	10.055	1465	1471	1487	rBV	755165	1023030	84.60%	10.764%
8	11.079	1634	1639	1654	rBV	711505	911219	75.36%	9.588%
9	12.024	1788	1794	1809	rBV	805608	1054365	87.19%	11.094%
10	13.286	1998	2001	2007	rVB4	15747	23747	1.96%	0.250%
11	13.414	2016	2022	2030	rBV10	20887	57869	4.79%	0.609%
12	13.512	2034	2038	2042	rBV6	7084	13508	1.12%	0.142%
13	13.585	2047	2050	2054	rBV5	9416	15653	1.29%	0.165%
14	13.670	2061	2064	2069	rBV7	11474	18857	1.56%	0.198%
15	13.798	2082	2085	2089	rBV2	18360	21738	1.80%	0.229%
16	13.847	2089	2093	2100	rBV5	22641	41748	3.45%	0.439%
17	13.926	2102	2106	2111	rVV7	13115	21390	1.77%	0.225%
18	14.012	2117	2120	2125	rBV7	8610	14027	1.16%	0.148%
19	14.067	2125	2129	2132	rBV5	26254	37466	3.10%	0.394%
20	14.170	2142	2146	2150	rBV5	15124	25780	2.13%	0.271%
21	14.225	2150	2155	2159	rBV4	57547	103907	8.59%	1.093%
22	14.323	2167	2171	2176	rBV6	17542	42831	3.54%	0.451%
23	14.481	2193	2197	2204	rVB5	69863	113511	9.39%	1.194%
24	14.554	2205	2209	2211	rBV2	23912	37430	3.10%	0.394%
25	14.615	2216	2219	2225	rVV2	106983	169704	14.03%	1.786%
26	14.670	2225	2228	2232	rVV	79244	90731	7.50%	0.955%
27	14.725	2233	2237	2239	rVV4	26193	39119	3.24%	0.412%
28	14.755	2239	2242	2245	rVV4	44457	50395	4.17%	0.530%
29	14.786	2245	2247	2250	rVV4	19638	25618	2.12%	0.270%
30	14.816	2250	2252	2254	rVV3	24827	24823	2.05%	0.261%
31	14.847	2254	2257	2263	rVB5	59338	72345	5.98%	0.761%
32	14.914	2265	2268	2272	rBV3	38016	58870	4.87%	0.619%
33	15.042	2284	2289	2294	rBV4	51739	103034	8.52%	1.084%
34	15.182	2307	2312	2315	rBV2	86363	150242	12.42%	1.581%
35	15.249	2320	2323	2331	rVB7	47140	89278	7.38%	0.939%
36	15.316	2331	2334	2340	rVB6	34448	60134	4.97%	0.633%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20071

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\82X031023W.M
Title : SW846 8260

37	15.377	2340	2344	2347	rBV4	69981	98786	8.17%	1.039%
38	15.414	2347	2350	2354	rVB4	41786	48192	3.99%	0.507%
39	15.481	2358	2361	2364	rBV3	46071	71478	5.91%	0.752%
40	15.560	2370	2374	2378	rVB2	200175	284640	23.54%	2.995%
41	15.609	2379	2382	2386	rVB3	59905	87026	7.20%	0.916%
42	15.853	2418	2422	2430	rBV7	56377	124811	10.32%	1.313%
43	15.944	2434	2437	2440	rBV4	29682	50296	4.16%	0.529%
44	16.091	2457	2461	2467	rBV7	51640	89244	7.38%	0.939%
45	16.280	2487	2492	2502	rVB4	68236	208961	17.28%	2.199%
46	16.426	2510	2516	2517	rBV4	45674	89200	7.38%	0.939%

Sum of corrected areas: 9504209

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ClientSampleId :
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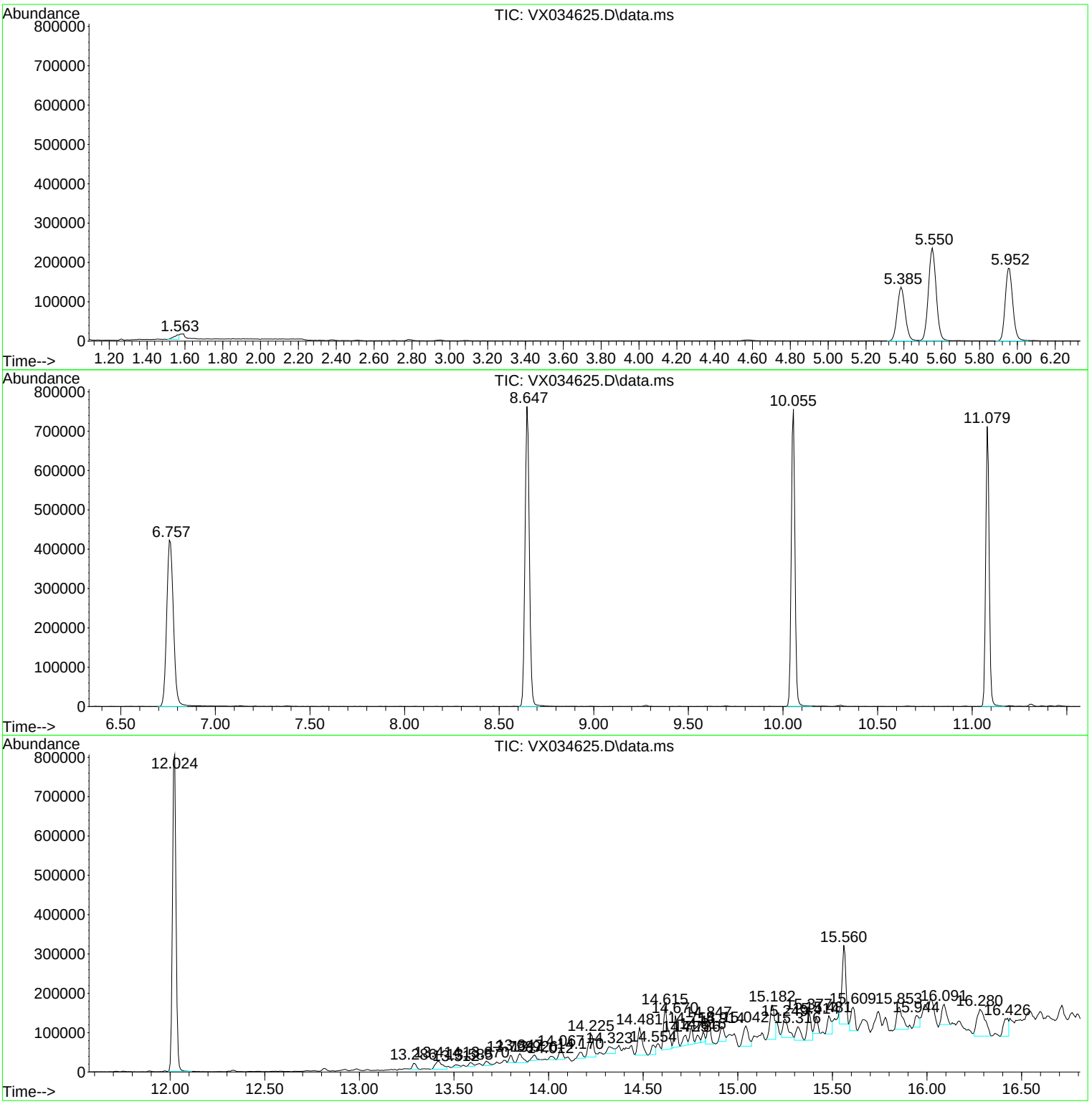
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
Data File : VX034625.D
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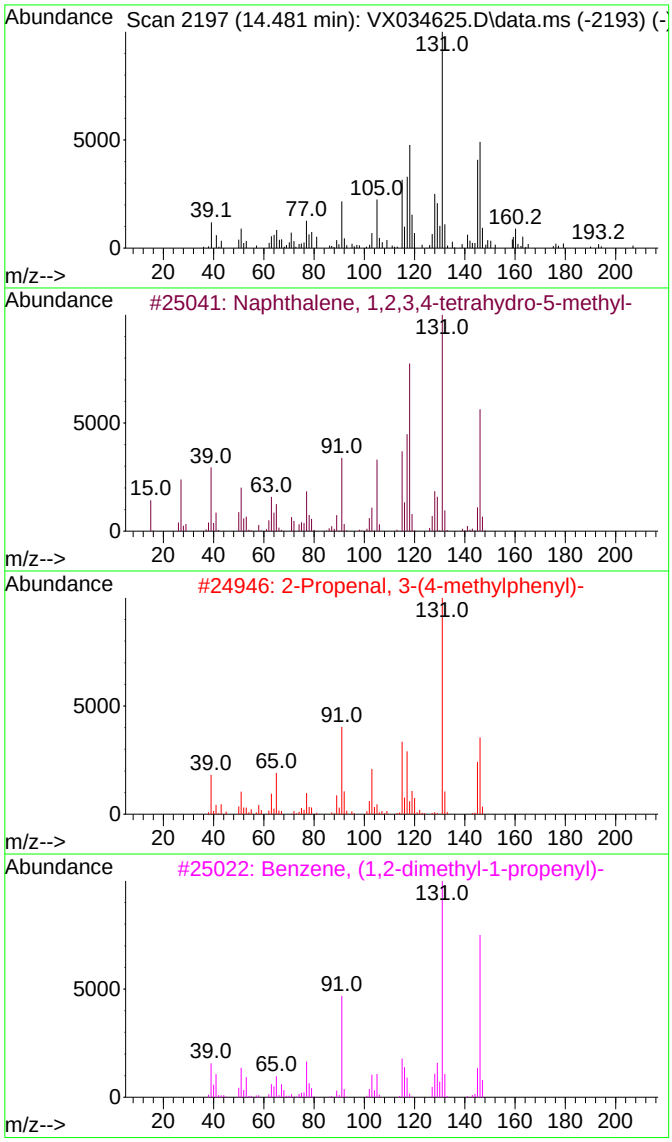
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

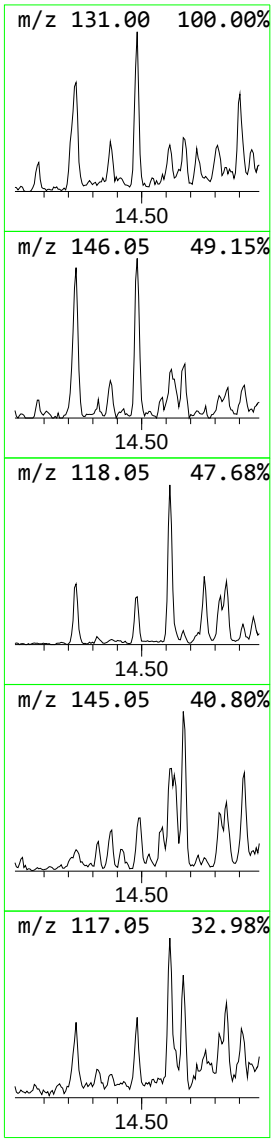
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	5.38 ug/l	113511	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
2	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	70
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	58
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	53
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	53





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Instrument :
MSVOA_X
ClientSampleId :
20071

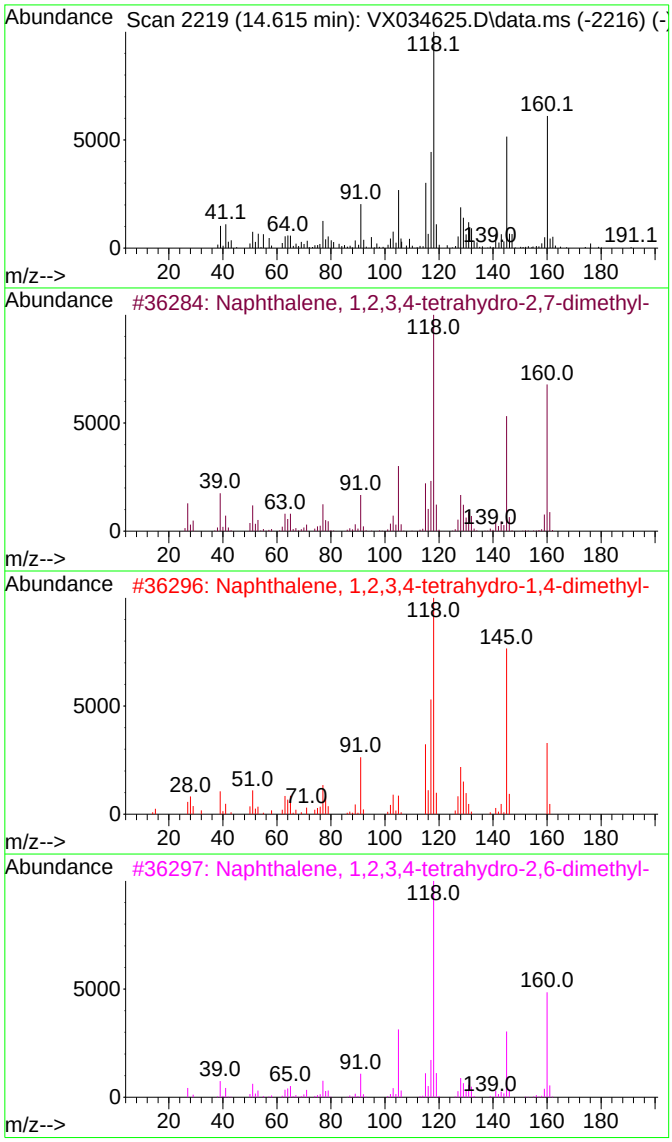
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

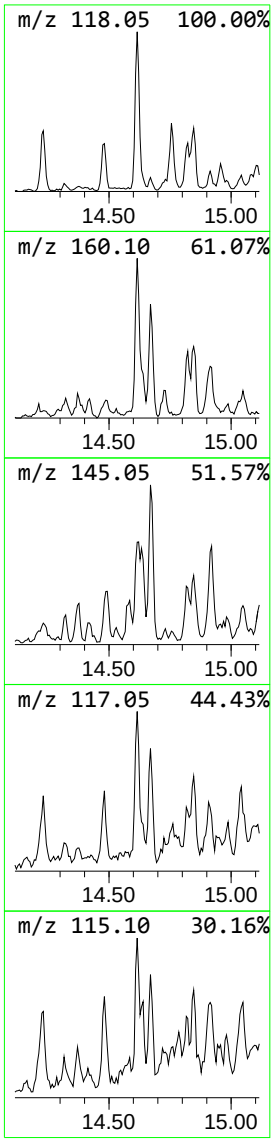
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	8.05 ug/l	169704	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	91
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	87
4	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	76
5	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	64





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Data File : VX034625.D
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Instrument :
MSVOA_X
ClientSampleId :
20071

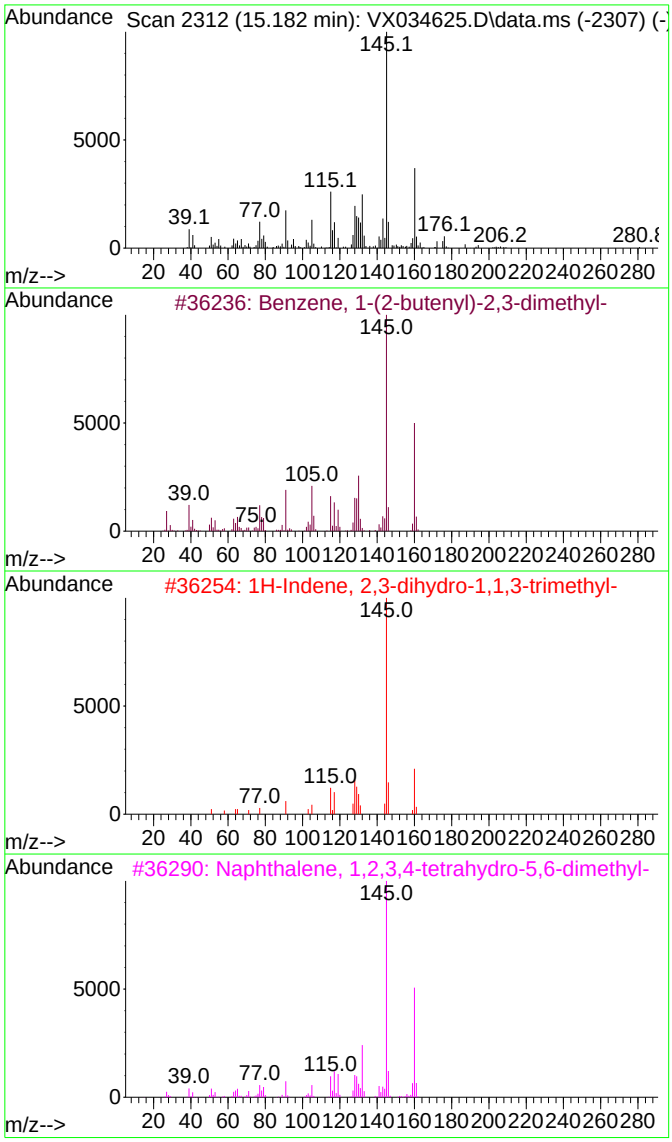
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

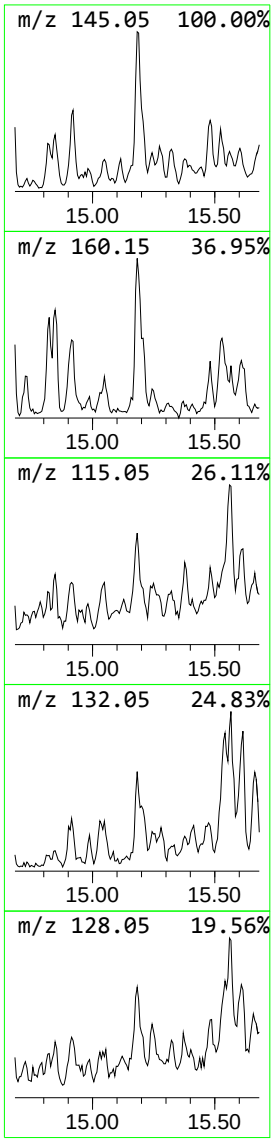
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-(2-butenyl)-2,3-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	7.12 ug/l	150242	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	91
2	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	89
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	87
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	83
5	1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	76





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Instrument :
MSVOA_X
ClientSampleId :
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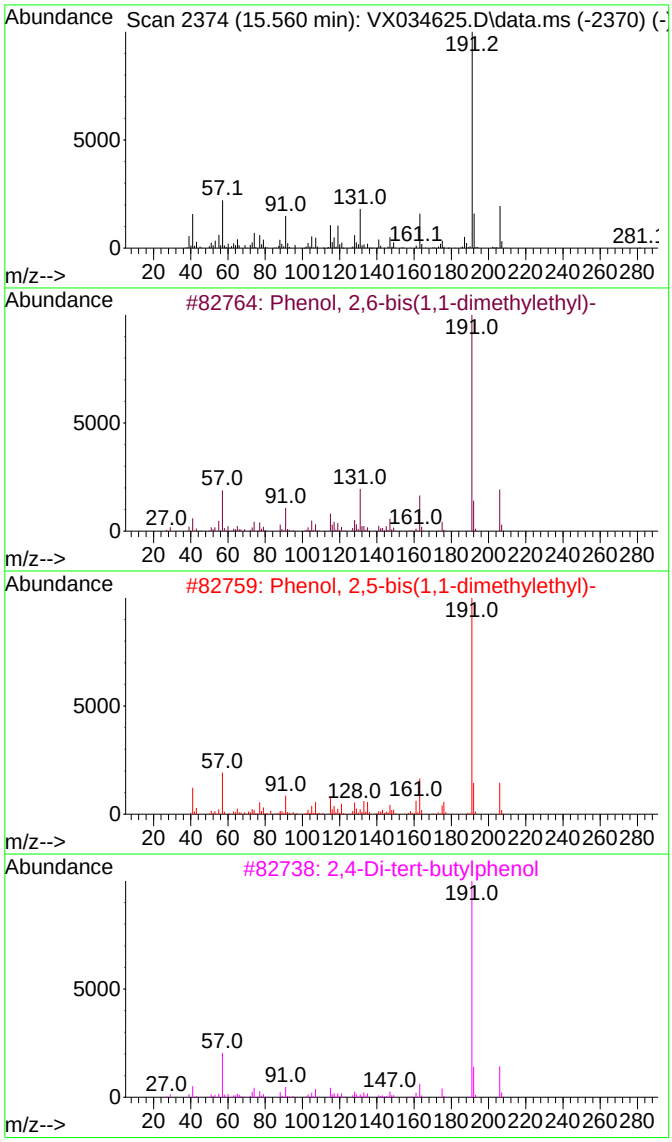
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

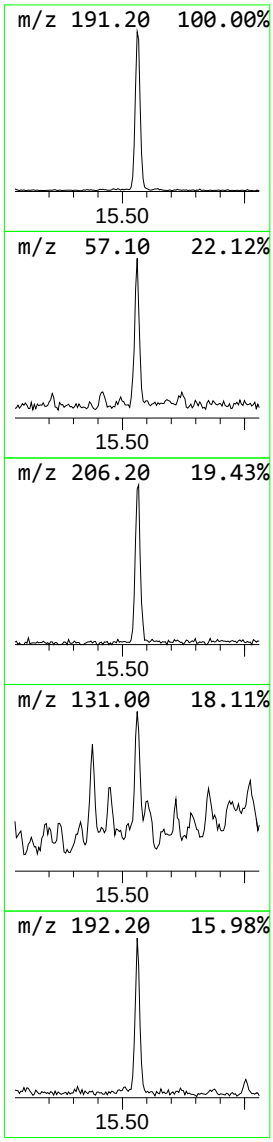
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	13.50 ug/l	284640	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	74
3	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	74
4	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	72
5	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	68





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Quant Title : SW846 8260

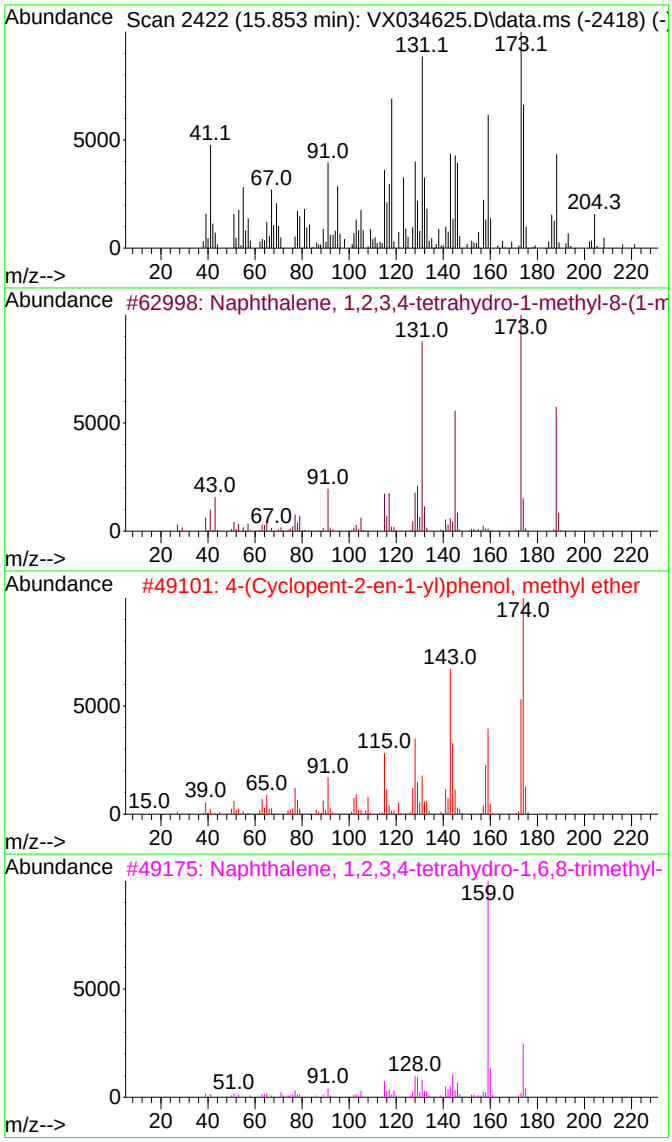
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

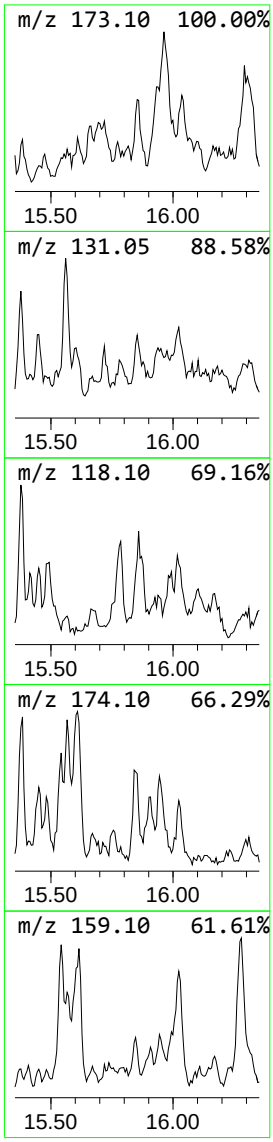
****

Peak Number 5 unknown15.853 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.853	5.92 ug/l	124811	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	188	C14H20	081603-43-2	46
2	4-(Cyclopent-2-en-1-yl)phenol, m...	174	C12H14O	031169-38-7	38
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	35
4	Methyl (Z)-2-(6-methylisobenzofu...	204	C12H12O3	1000481-36-4	30
5	Propanoic acid, 2-[4-(1-buten-3-...	204	C13H16O2	1010162-33-3	25





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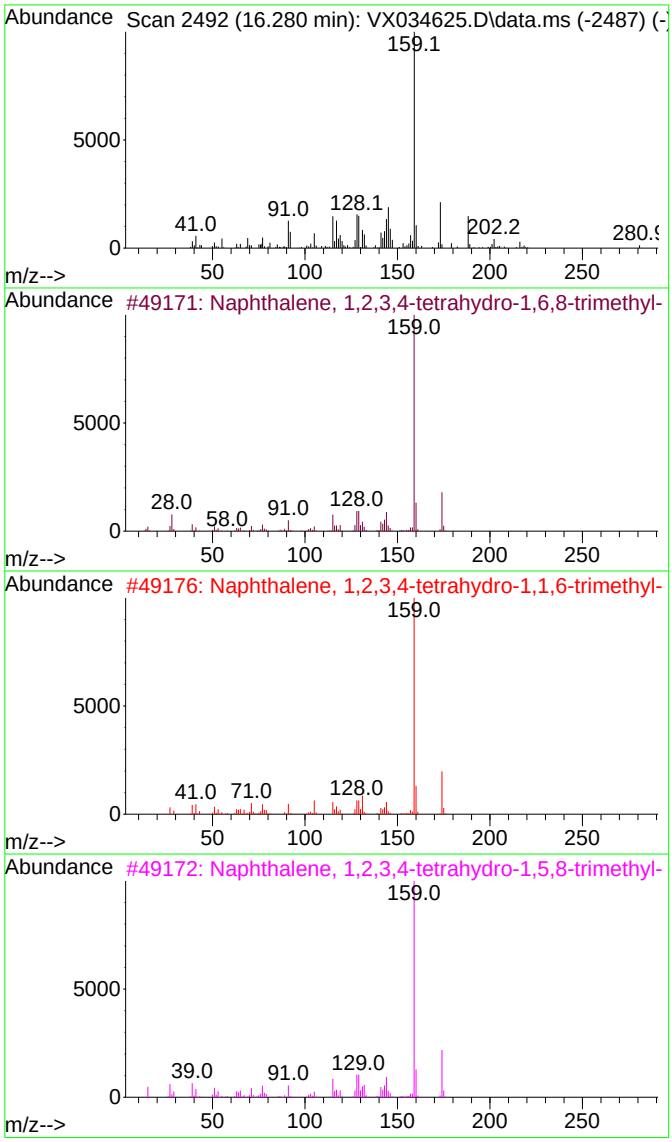
Quant Title : SW846 8260

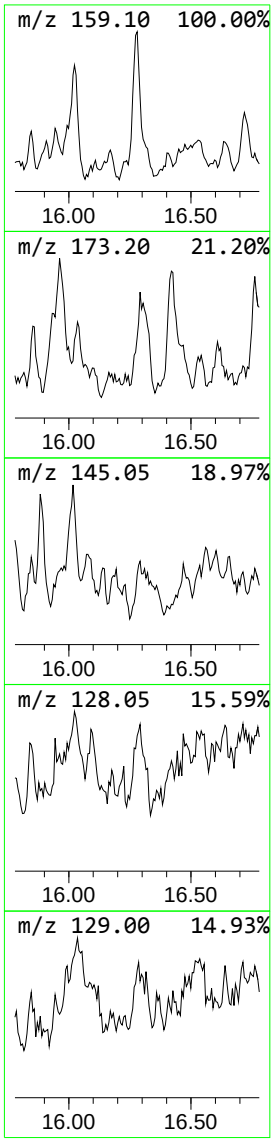
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.279	9.91 ug/l	208961	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	92
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-55-0	70
5	cis-Calamenene	202	C15H22	072937-55-4	70





Tentatively Identified Compound (LSC) summary

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MSVOA_X
ClientSampleId :
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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
Naphthalene, 1,...	14.481	5.4	ug/l	113511	4	12.024	1054370	50.0
Naphthalene, 1,...	14.615	8.1	ug/l	169704	4	12.024	1054370	50.0
Benzene, 1-(2-b...	15.182	7.1	ug/l	150242	4	12.024	1054370	50.0
Phenol, 2,6-bis...	15.560	13.5	ug/l	284640	4	12.024	1054370	50.0
unknown15.853	15.853	5.9	ug/l	124811	4	12.024	1054370	50.0
Naphthalene, 1,...	16.279	9.9	ug/l	208961	4	12.024	1054370	50.0