LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039214.D
Acq On : 14 Dec 2023 17:28
Operator : JC/MD
Sample : 05829-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13D

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\82X121323W.M
Title : SW846 8260

Signal : TIC: VX039214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	42	rBV	25267	67856	8.38%	1.116%
2	5.385	693	705	719	rBV2	82866	244927	30.25%	4.028%
3	5.549	721	732	748	rVB	123056	355958	43.96%	5.855%
4	5.952	788	798	808	rBV	97423	258610	31.94%	4.253%
5	6.037	808	812	823	rVB3	7374	19595	2.42%	0.322%
6	6.756	921	930	949	rBV	228021	549038	67.80%	9.030%
7	8.646	1234	1240	1257	rVB	473722	759322	93.77%	12.489%
8	9.274	1337	1343	1350	rBV5	7375	11872	1.47%	0.195%
9	10.055	1465	1471	1488	rVB	537745	752917	92.98%	12.383%
10	10.195	1488	1494	1503	rVB	34087	48241	5.96%	0.793%
11	10.305	1505	1512	1517	rBV4	5620	9014	1.11%	0.148%
12	10.640	1563	1567	1578	rVB	6801	10532	1.30%	0.173%
13	10.963	1615	1620	1626	rBV	8944	11711	1.45%	0.193%
14	11.079	1634	1639	1651	rBV	472444	613071	75.71%	10.083%
15	11.304	1672	1676	1682	rBV2	6283	8347	1.03%	0.137%
16	11.402	1684	1692	1697	rBV	5382	8624	1.06%	0.142%
17	11.609	1721	1726	1733	rBV	37623	49454	6.11%	0.813%
18	11.749	1744	1749	1756	rVB	44255	57416	7.09%	0.944%
19	12.018	1788	1793	1800	rBV	633287	809775	100.00%	13.319%
20	12.085	1800	1804	1810	rVB	33740	43970	5.43%	0.723%
21	12.243	1821	1830	1837	rBV2	47789	66577	8.22%	1.095%
22	12.310	1837	1841	1848	rVB3	10304	16524	2.04%	0.272%
23	12.414	1854	1858	1863	rVB	7927	10565	1.30%	0.174%
24	12.530	1871	1877	1879	rBV	8011	10466	1.29%	0.172%
25	12.609	1886	1890	1894	rBV2	9645	12924	1.60%	0.213%
26	12.694	1899	1904	1911	rBV	29420	43846	5.41%	0.721%
27	12.847	1923	1929	1935	rBV6	6291	13134	1.62%	0.216%
28	12.920	1937	1941	1944	rVV	11271	14378	1.78%	0.236%
29	12.963	1944	1948	1954	rVB	15051	19619	2.42%	0.323%
30	13.170	1978	1982	1985	rVB2	10131	12225	1.51%	0.201%
31	13.286	1991	2001	2006	rBV2	30688	47612	5.88%	0.783%
32	13.341	2006	2010	2018	rVV2	27716	36363	4.49%	0.598%
33	13.420	2018	2023	2029	rVB	62523	84865	10.48%	1.396%
34	13.542	2039	2043	2046	rBV2	12475	16606	2.05%	0.273%
35	13.578	2046	2049	2057	rVB4	4790	8355	1.03%	0.137%
36	13.664	2057	2063	2068	rVB5	4085	8962	1.11%	0.147%

LSC Area Percent Report

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Title : SW846 8260

37	13.774	2072	2081	2090	rBV	208675	259671	32.07%	4.271%
38	14.133	2137	2140	2146	rVV7	3748	8395	1.04%	0.138%
39	14.219	2149	2154	2157	rBV2	11457	16911	2.09%	0.278%
40	14.316	2164	2170	2176	rBV3	16225	26695	3.30%	0.439%
41	14.517	2200	2203	2210	rVB2	5821	8390	1.04%	0.138%
42	14.633	2217	2222	2232	rBV	39876	53121	6.56%	0.874%
43	14.773	2240	2245	2251	rBV	161067	214258	26.46%	3.524%
44	15.206	2309	2316	2320	rBV	14685	21605	2.67%	0.355%
45	15.407	2345	2349	2354	rVB	11068	15639	1.93%	0.257%
46	15.474	2354	2360	2369	rBV	34574	54315	6.71%	0.893%
47	15.609	2376	2382	2393	rVB	61748	104260	12.88%	1.715%
48	15.834	2407	2419	2430	rBV	20956	54767	6.76%	0.901%
49	15.987	2438	2444	2454	rVB2	15095	26334	3.25%	0.433%
50	16.084	2456	2460	2468	rVV4	4854	8728	1.08%	0.144%
51	16.322	2492	2499	2511	rBV	47778	93663	11.57%	1.541%

Sum of corrected areas: 6080023

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MSVOA_X
ClientSampleId :
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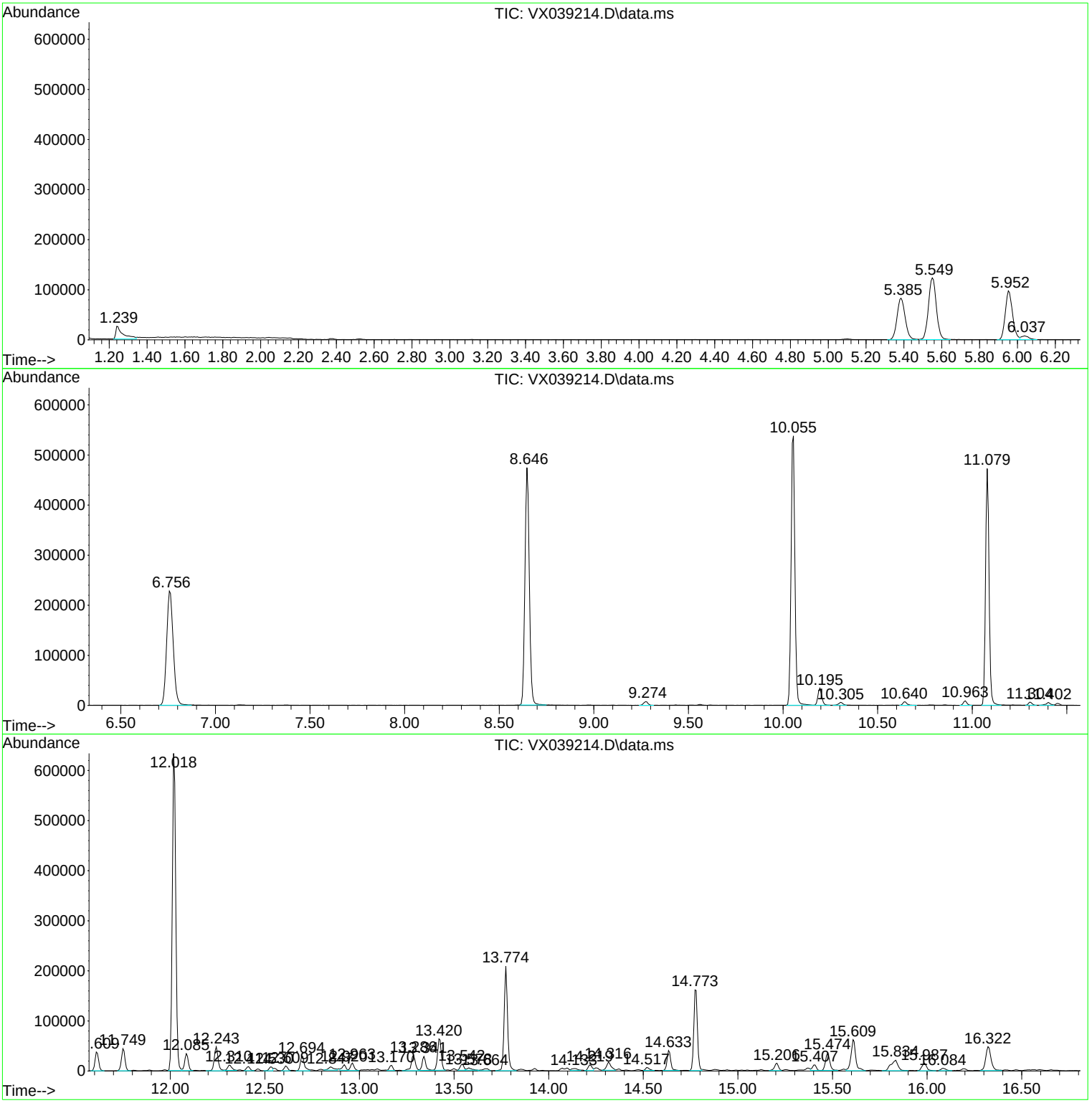
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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Data File : VX039214.D
Acq On : 14 Dec 2023 17:28
Operator : JC/MD
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

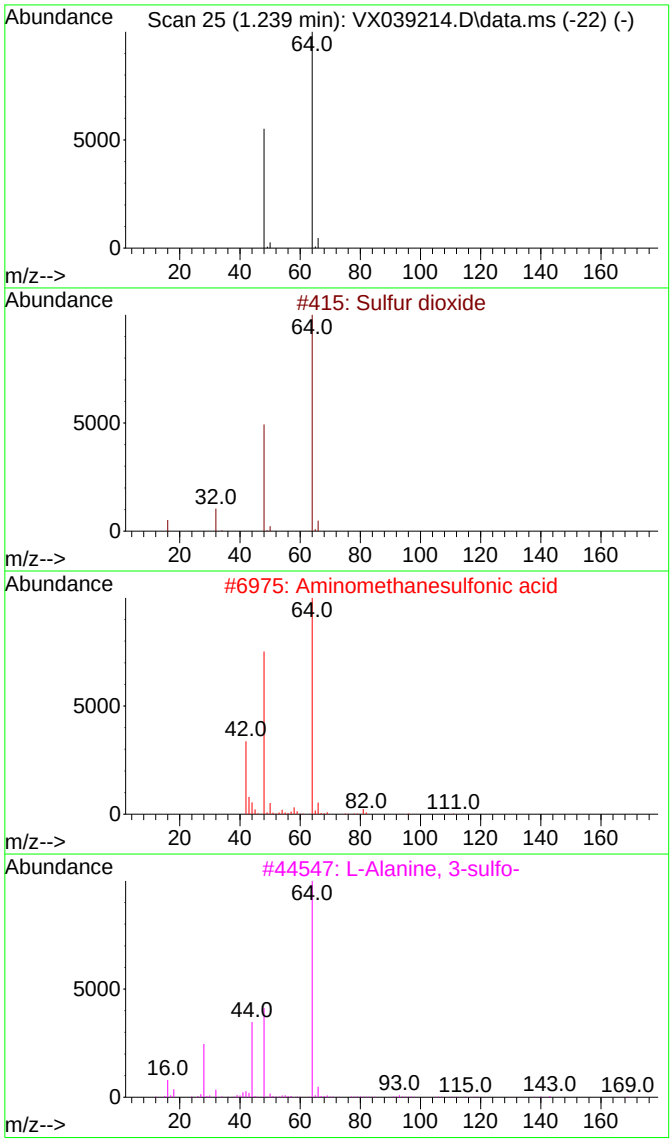
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

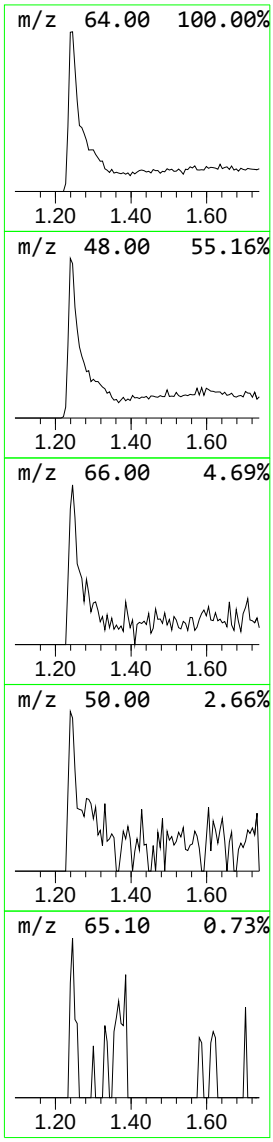
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	9.53 ug/l	67856	Pentafluorobenzene	5.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument :
MSVOA_X
ClientSampleId :
MW-13D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

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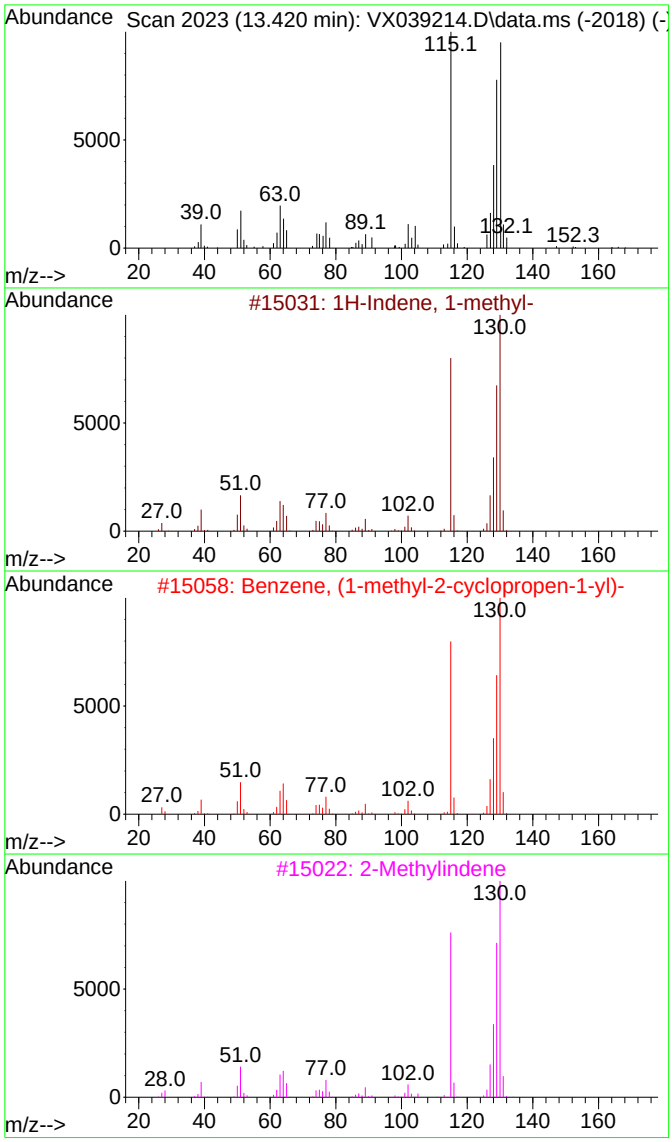
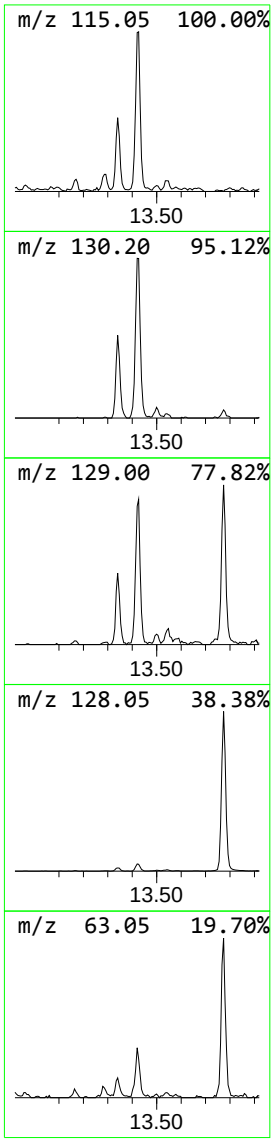
Peak Number 2 1H-Indene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	5.24 ug/l	84865	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3	2-Methylindene	130	C10H10	002177-47-1	96
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	93





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Instrument :
MSVOA_X
ClientSampleId :
MW-13D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

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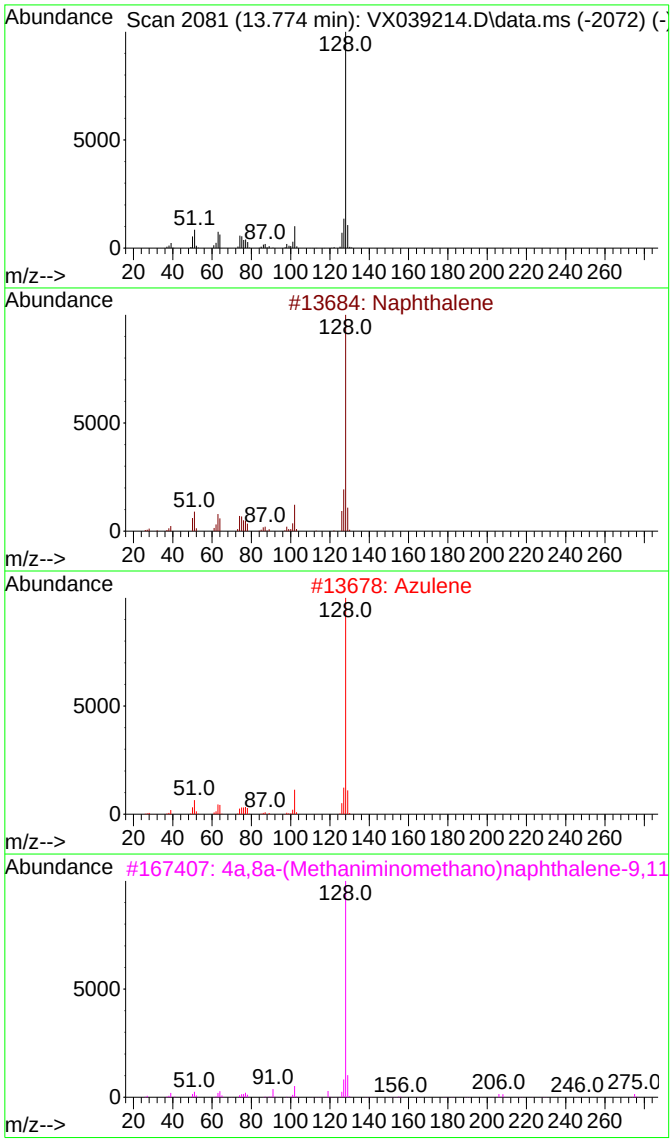
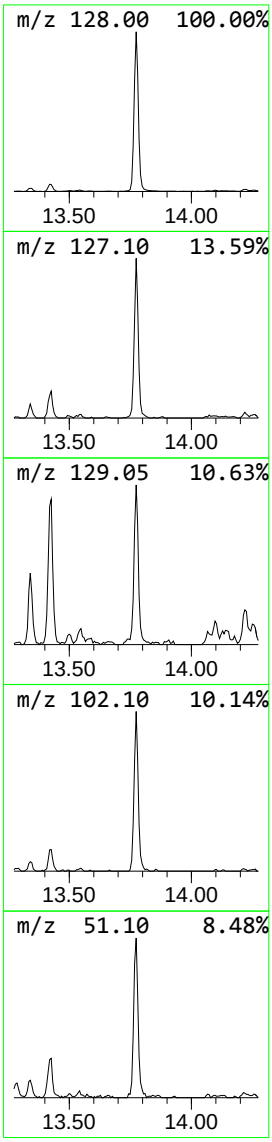
Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	16.03 ug/l	259671	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	97
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	72
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59





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Instrument :
MSVOA_X
ClientSampleId :
MW-13D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

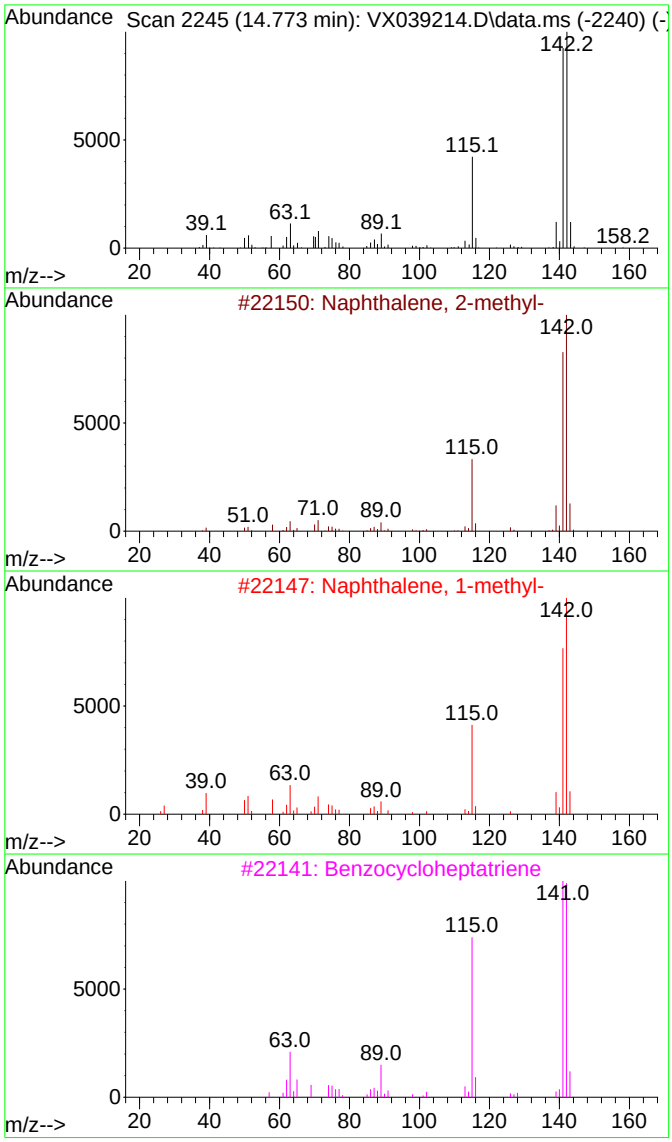
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

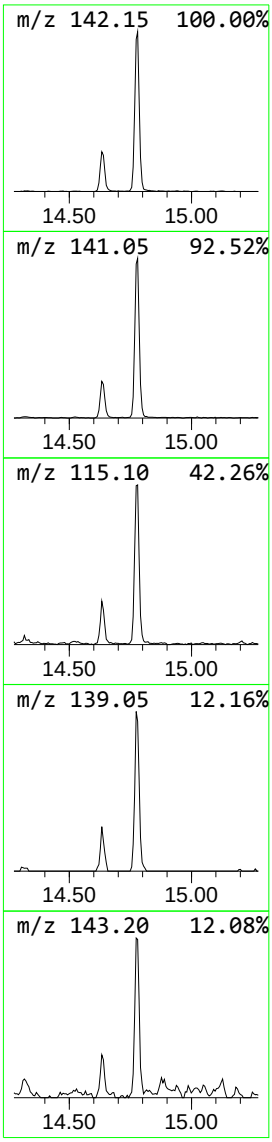
****

Peak Number 4 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.773	13.23 ug/l	214258	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	94
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





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Instrument :
MSVOA_X
ClientSampleId :
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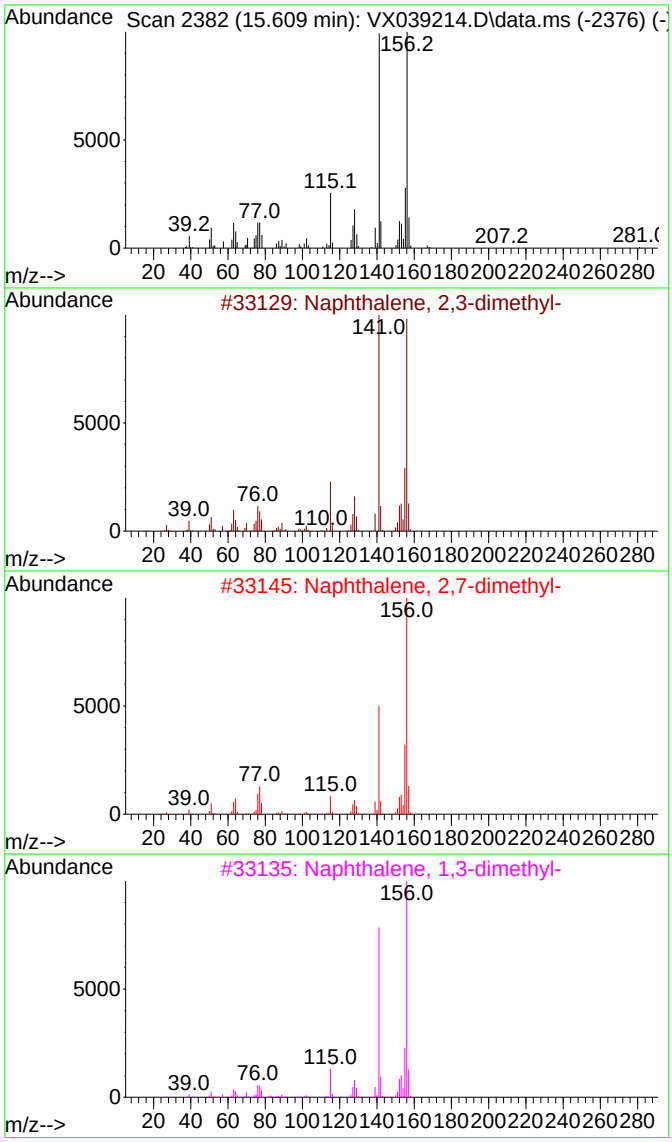
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

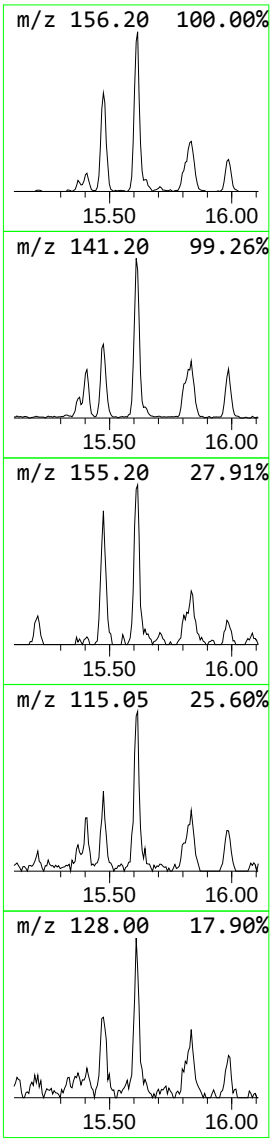
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.608	6.44 ug/l	104260	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97





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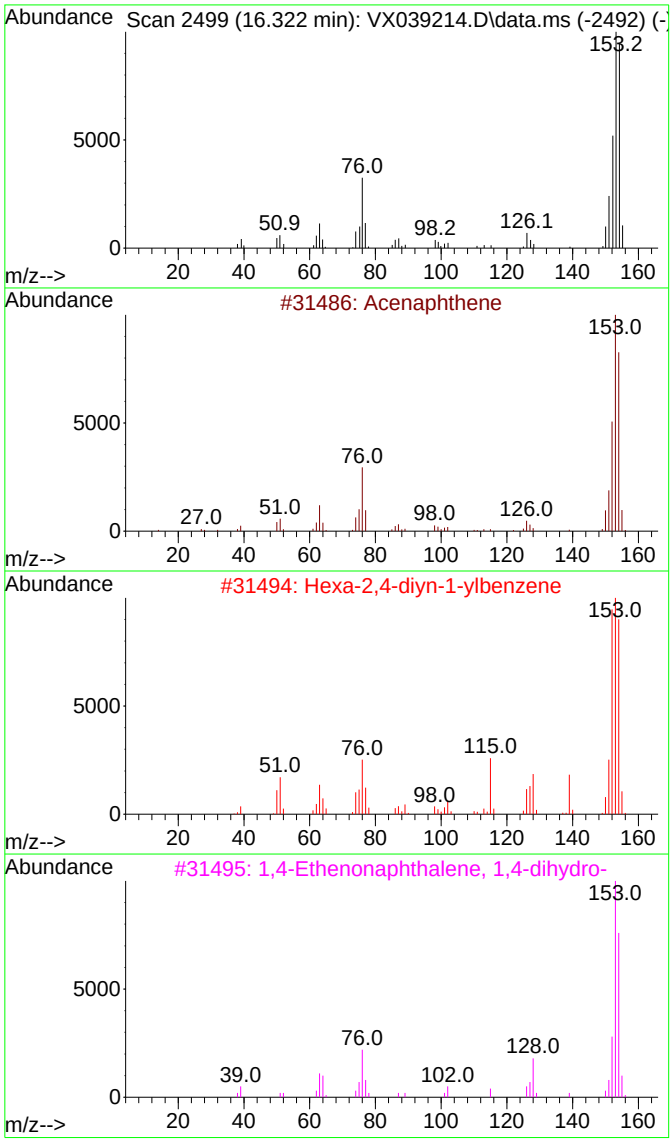
Quant Title : SW846 8260

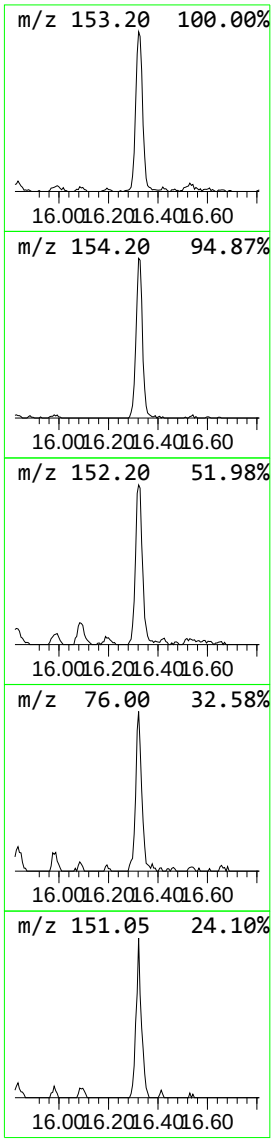
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	5.78 ug/l	93663	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	96
2	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	58
4	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	53
5	Biphenyl	154	C12H10	000092-52-4	47





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
Sulfur dioxide	1.239	9.5	ug/l	67856	1	5.549	355958	50.0
1H-Indene, 1-me...	13.420	5.2	ug/l	84865	4	12.018	809775	50.0
Azulene	13.774	16.0	ug/l	259671	4	12.018	809775	50.0
Benzocyclohepta...	14.773	13.2	ug/l	214258	4	12.018	809775	50.0
Naphthalene, 2,...	15.608	6.4	ug/l	104260	4	12.018	809775	50.0
Hexa-2,4-diyn-1...	16.322	5.8	ug/l	93663	4	12.018	809775	50.0