LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X112124W.M
Title : SW846 8260

Signal : TIC: VX044049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rBV	507107	535706	4.21%	0.666%
2	1.721	98	104	116	rVB	967515	1321025	10.39%	1.642%
3	1.886	126	131	135	rBV	95384	128142	1.01%	0.159%
4	1.935	135	139	153	rVV2	443563	804258	6.32%	1.000%
5	2.050	153	158	169	rVV	237548	347704	2.73%	0.432%
6	2.148	169	174	178	rVV	176899	256899	2.02%	0.319%
7	2.203	178	183	193	rVB	258574	404185	3.18%	0.502%
8	2.739	258	271	274	rBV	94910	233550	1.84%	0.290%
9	2.812	279	283	286	rVV	192421	372932	2.93%	0.464%
10	2.855	286	290	310	rVB2	250982	576491	4.53%	0.717%
11	3.093	320	329	346	rVB2	145927	354293	2.79%	0.440%
12	3.434	376	385	398	rVB2	88747	200732	1.58%	0.250%
13	4.294	516	526	539	rVB	274278	778916	6.13%	0.968%
14	5.184	662	672	683	rVB3	41592	134528	1.06%	0.167%
15	5.379	692	704	711	rBV2	87259	277064	2.18%	0.344%
16	5.464	711	718	725	rVV3	101839	320097	2.52%	0.398%
17	5.544	725	731	739	rVB	99270	258805	2.04%	0.322%
18	5.818	765	776	788	rBV3	43740	139869	1.10%	0.174%
19	5.952	788	798	802	rVV2	108533	260274	2.05%	0.324%
20	6.031	802	811	823	rVV	1738419	4636527	36.46%	5.764%
21	6.190	824	837	843	rVV4	78336	336043	2.64%	0.418%
22	6.245	843	846	855	rVV4	55312	147025	1.16%	0.183%
23	6.757	922	930	940	rBV	227161	579248	4.56%	0.720%
24	7.373	1018	1031	1046	rBV4	158105	426096	3.35%	0.530%
25	8.500	1209	1216	1224	rVB3	69376	134363	1.06%	0.167%
26	8.647	1234	1240	1246	rVB	443164	691420	5.44%	0.860%
27	8.714	1246	1251	1258	rBV	374177	566659	4.46%	0.704%
28	8.952	1281	1290	1297	rBV	142092	250364	1.97%	0.311%
29	9.043	1297	1305	1311	rVB2	154170	251517	1.98%	0.313%
30	10.049	1461	1470	1475	rBV	443798	669454	5.26%	0.832%
31	10.195	1488	1494	1504	rBV	9516143	12716648	100.00%	15.809%
32	10.299	1506	1511	1524	rVB	3133061	4123624	32.43%	5.126%
33	10.640	1562	1567	1582	rVB	1367305	1900597	14.95%	2.363%
34	10.957	1614	1619	1626	rBV	313065	414663	3.26%	0.515%
35	11.079	1634	1639	1645	rBV	382806	479642	3.77%	0.596%
36	11.305	1668	1676	1682	rBV	665213	859238	6.76%	1.068%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X112124W.M
Title : SW846 8260

37	11.396	1682	1691	1696	rVV	1029992	1235556	9.72%	1.536%
38	11.610	1721	1726	1737	rBV	4578812	5448689	42.85%	6.774%
39	11.750	1744	1749	1755	rVB	6441578	7451272	58.59%	9.263%
40	12.018	1788	1793	1797	rBV2	495153	660141	5.19%	0.821%
41	12.085	1799	1804	1809	rVB	5556437	6499086	51.11%	8.079%
42	12.244	1824	1830	1837	rBV	5622285	6907586	54.32%	8.587%
43	12.311	1837	1841	1849	rVB2	307051	434544	3.42%	0.540%
44	12.408	1852	1857	1862	rBV	873786	1095356	8.61%	1.362%
45	12.463	1862	1866	1872	rVB	268653	345091	2.71%	0.429%
46	12.530	1872	1877	1880	rBV	638610	835668	6.57%	1.039%
47	12.609	1885	1890	1894	rBV	1052980	1300127	10.22%	1.616%
48	12.646	1894	1896	1900	rVB	230393	225268	1.77%	0.280%
49	12.695	1900	1904	1913	rBV2	793665	1138480	8.95%	1.415%
50	12.847	1923	1929	1934	rVB	341440	424542	3.34%	0.528%
51	12.920	1934	1941	1944	rBV	608680	731970	5.76%	0.910%
52	12.963	1944	1948	1954	rVB	576308	713976	5.61%	0.888%
53	13.164	1977	1981	1986	rVB	622559	736277	5.79%	0.915%
54	13.292	1997	2002	2007	rVB2	1628515	2153455	16.93%	2.677%
55	13.420	2019	2023	2031	rVB	313556	400107	3.15%	0.497%
56	13.585	2046	2050	2055	rVB3	97631	167582	1.32%	0.208%
57	13.664	2060	2063	2069	rVB2	113683	173687	1.37%	0.216%
58	13.774	2074	2081	2087	rBV	2857047	3456108	27.18%	4.297%
59	13.865	2091	2096	2101	rVB	387456	487811	3.84%	0.606%
60	14.780	2240	2246	2254	rBV	392547	528589	4.16%	0.657%

Sum of corrected areas: 80439566

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
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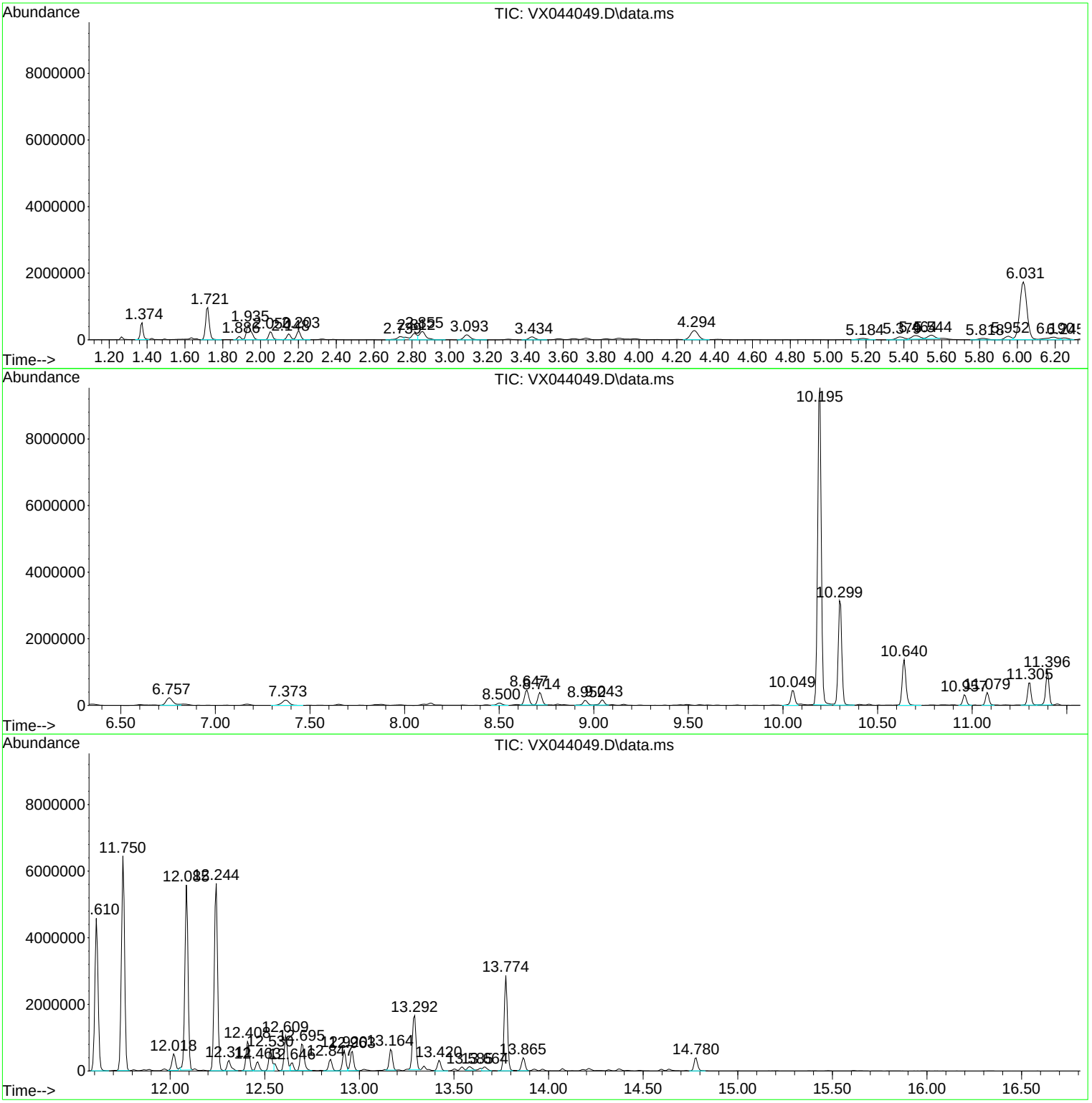
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

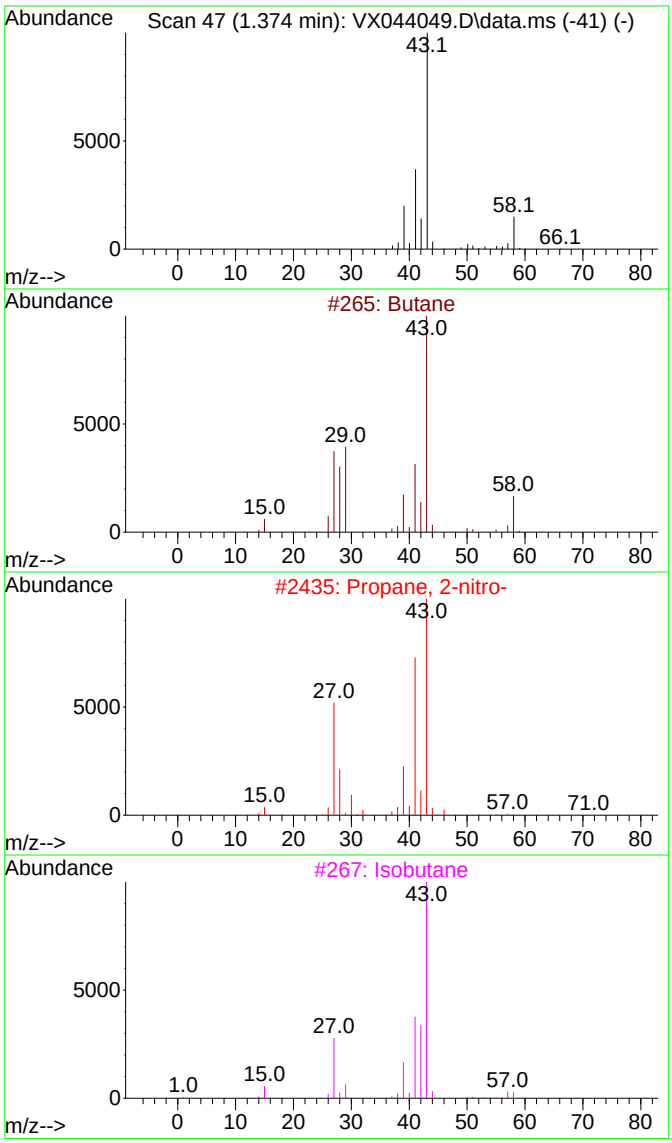
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

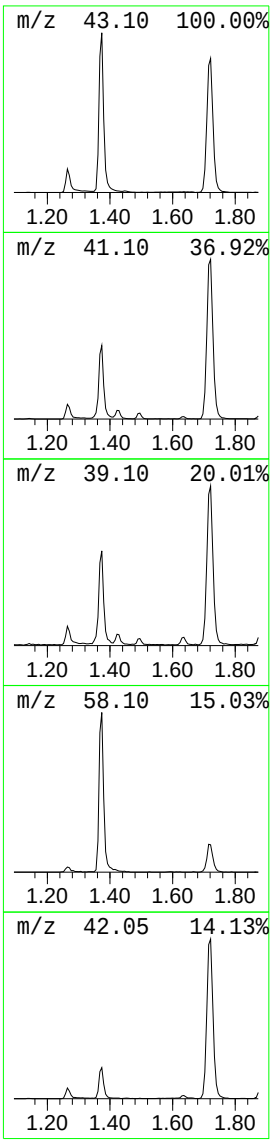
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	103.50 ug/l	535706	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

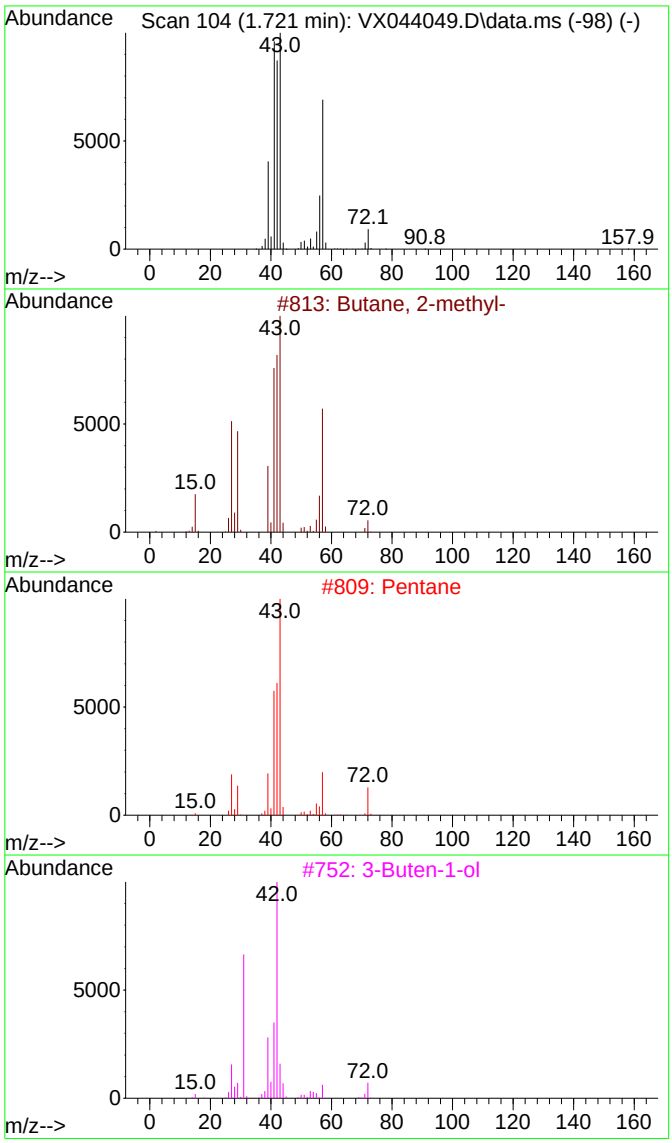
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

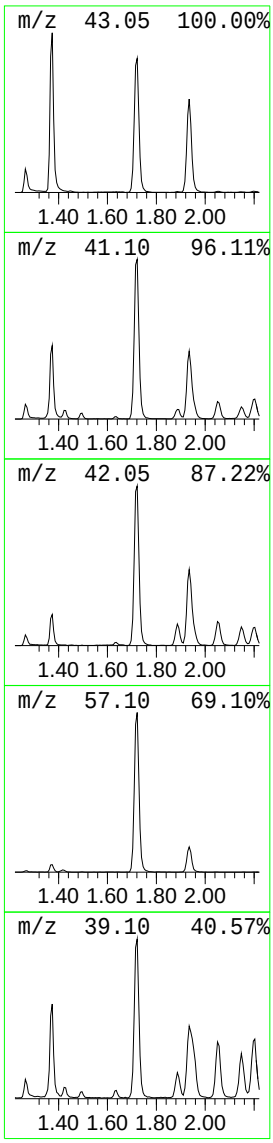
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.721	255.22 ug/l	1321030	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	1-Butene	56	C4H8	000106-98-9	27
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

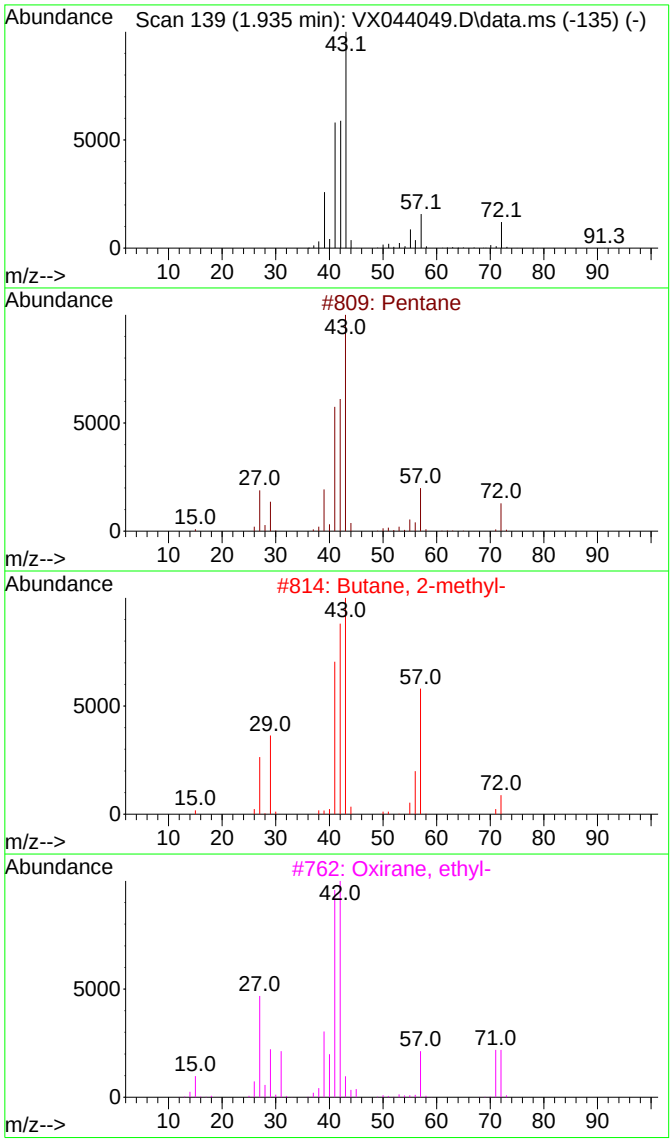
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

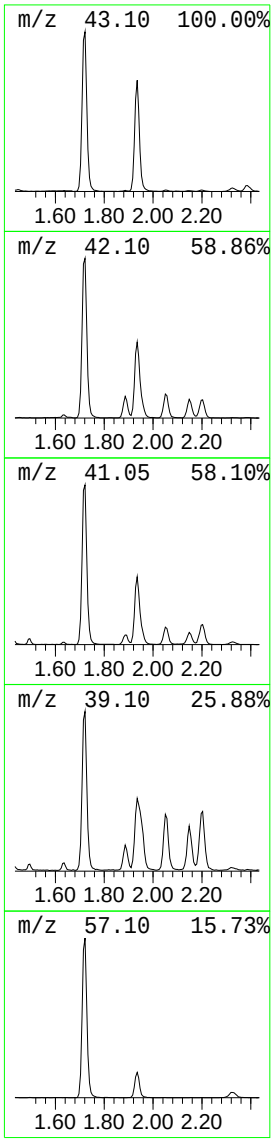
****

Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.935	155.38 ug/l	804258	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4	Tetrahydrofuran	72	C4H8O	000109-99-9	38
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

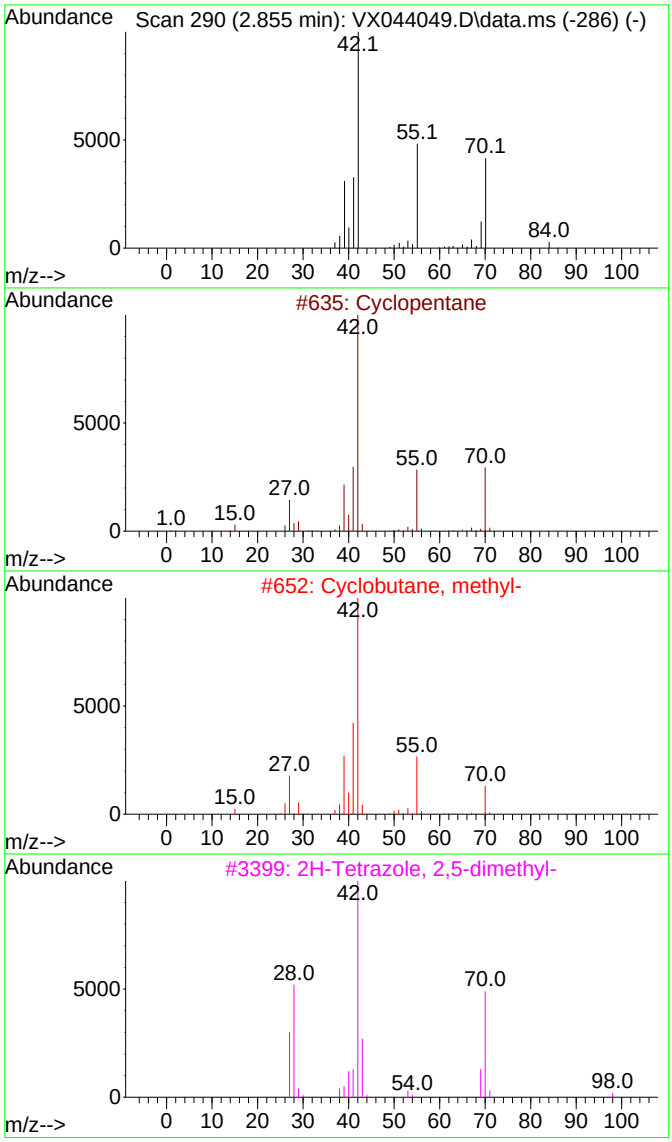
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

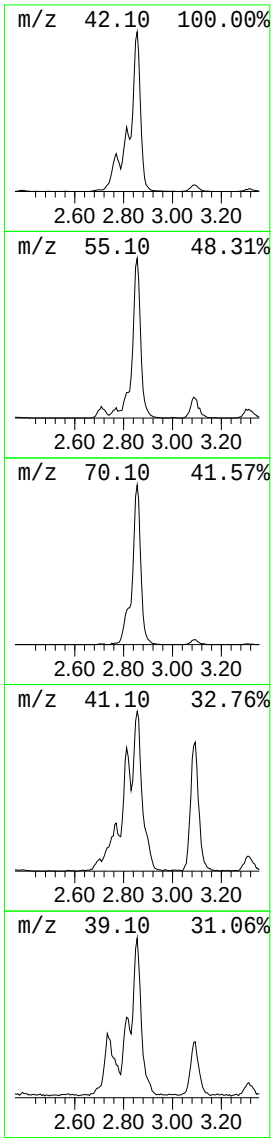
****

Peak Number 4 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.855	111.38 ug/l	576491	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	56
4	1-Pentene	70	C5H10	000109-67-1	50
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

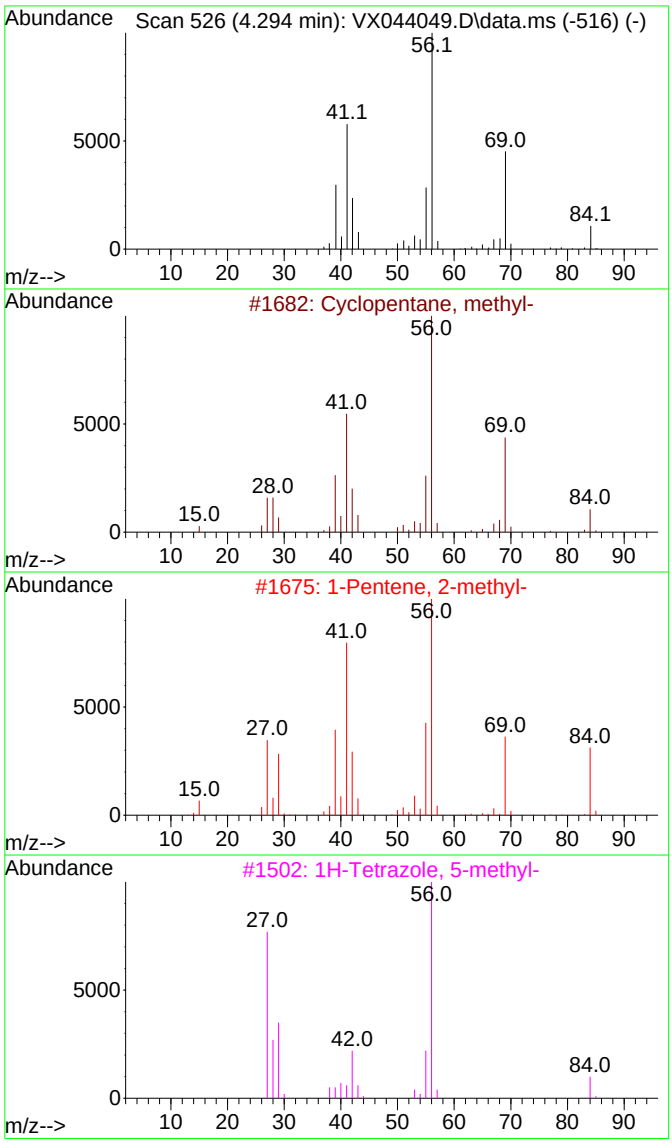
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

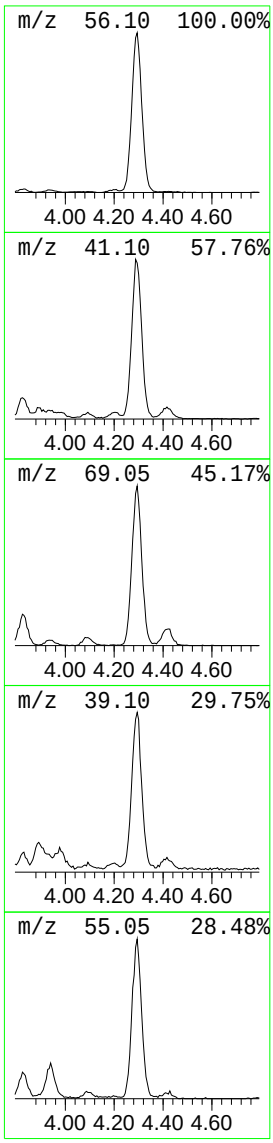
****

Peak Number 5 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	150.48 ug/l	778916	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclohexane	84	C6H12	000110-82-7	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

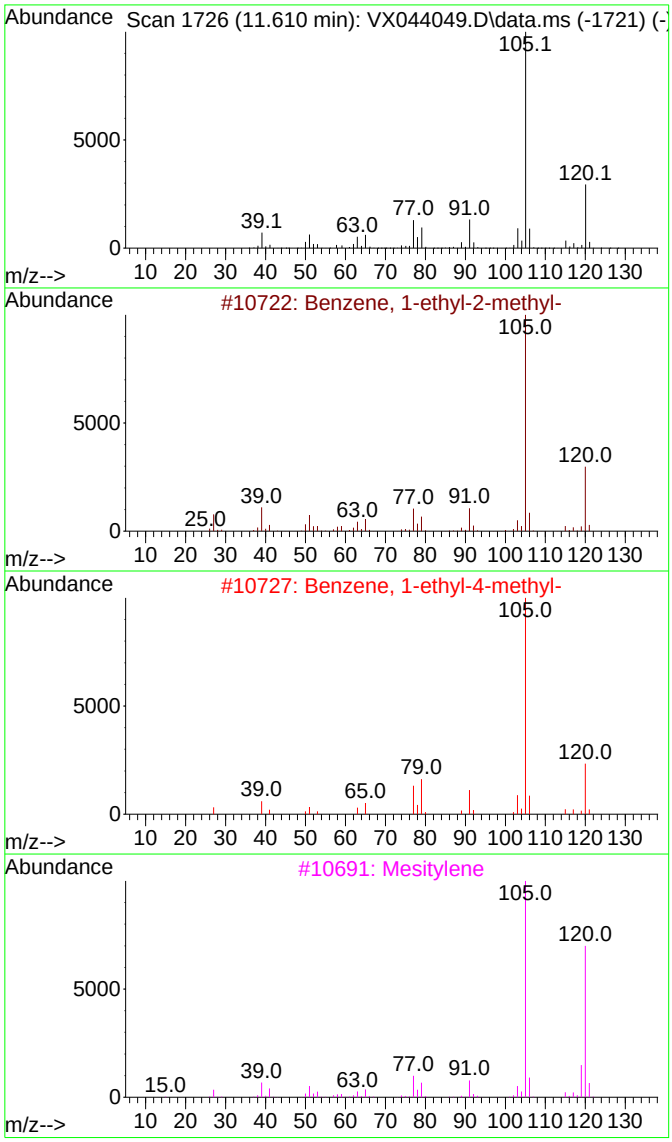
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

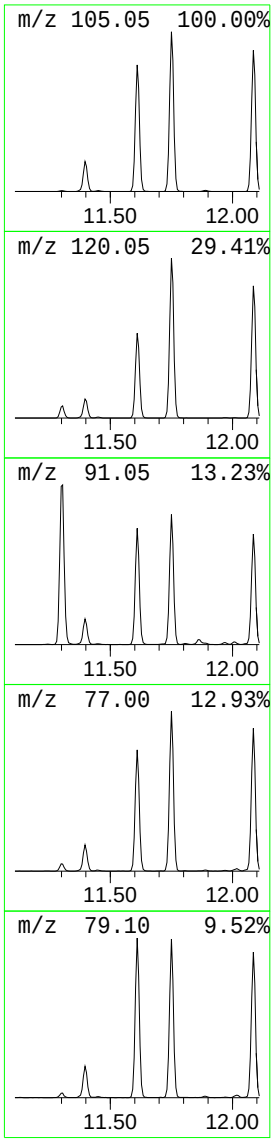
****

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	412.69 ug/l	5448690	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

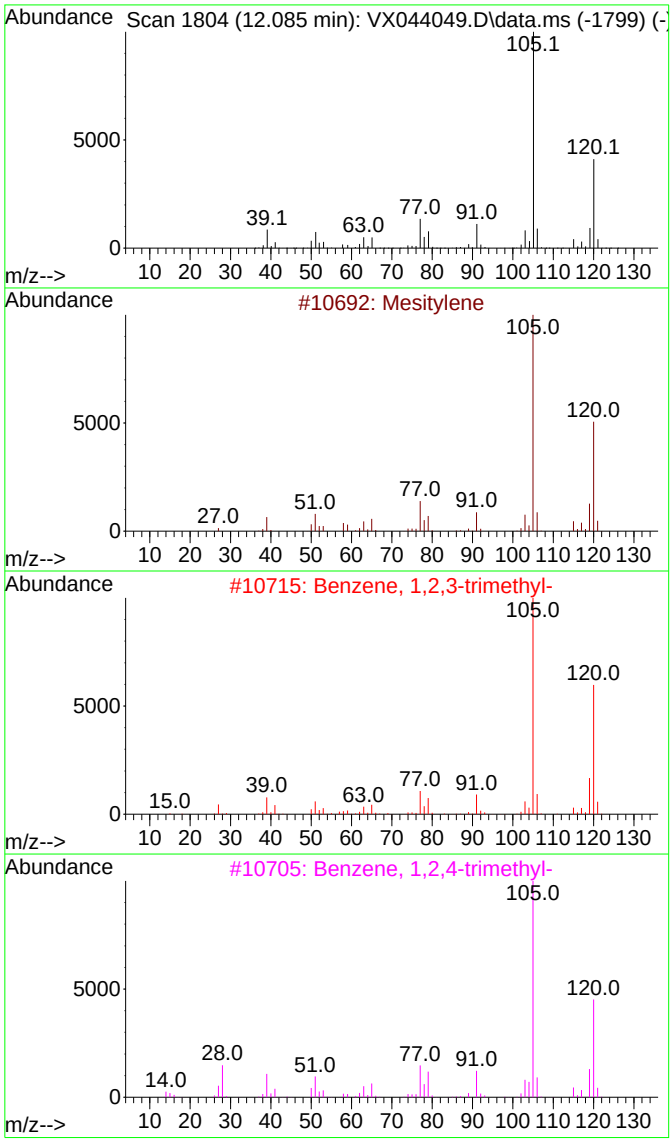
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

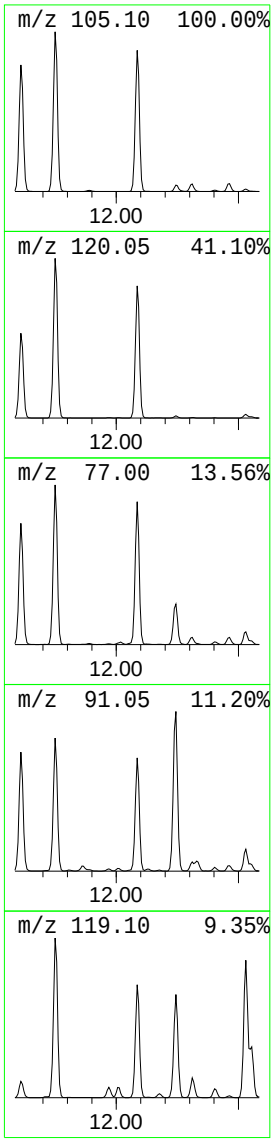
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	492.25 ug/l	6499090	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

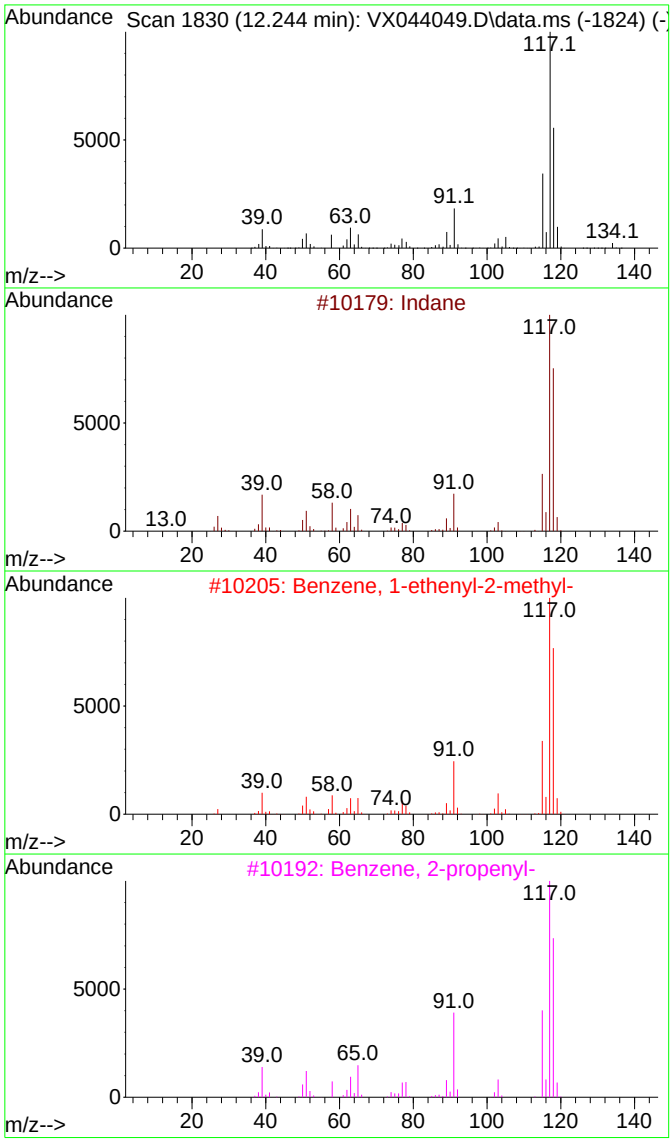
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

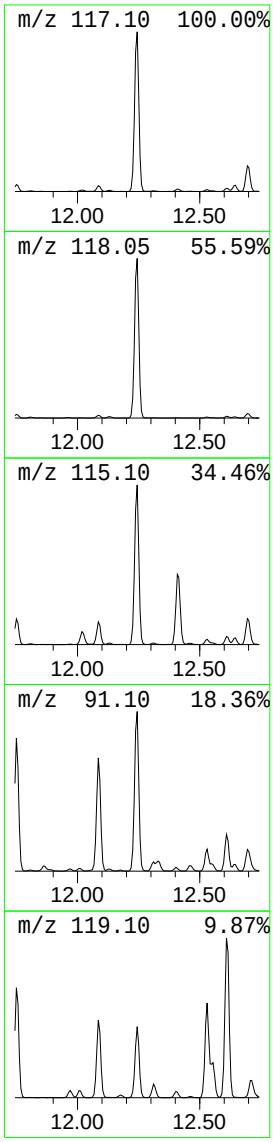
****

Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	523.19 ug/l	6907590	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	89
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80





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Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

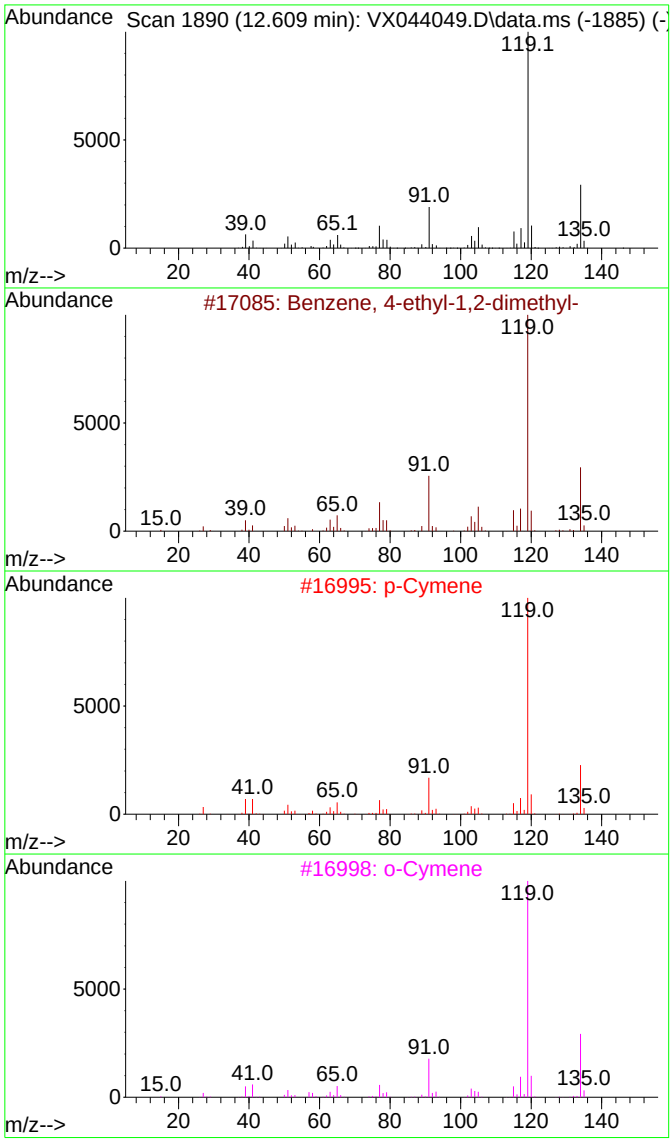
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

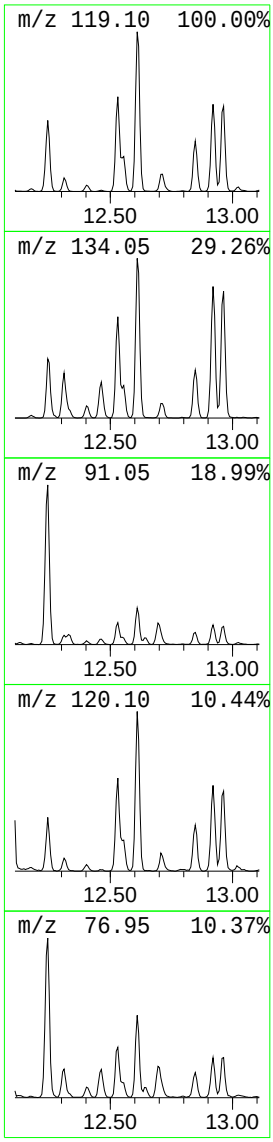
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	98.47 ug/l	1300130	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	p-Cymene	134	C10H14	000099-87-6	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

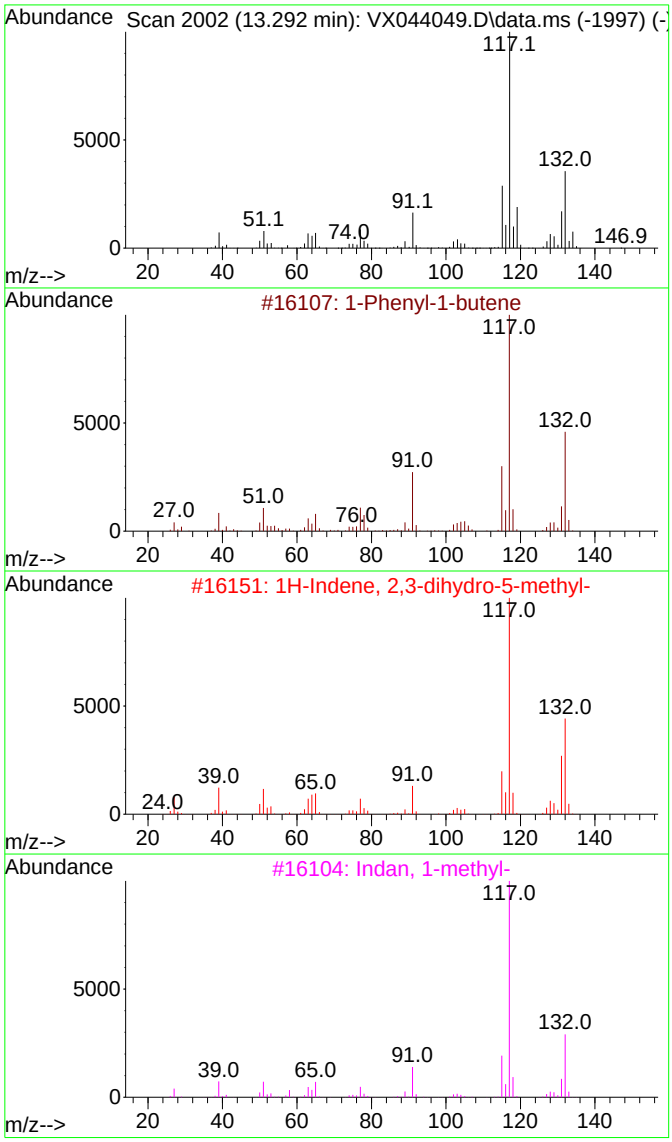
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

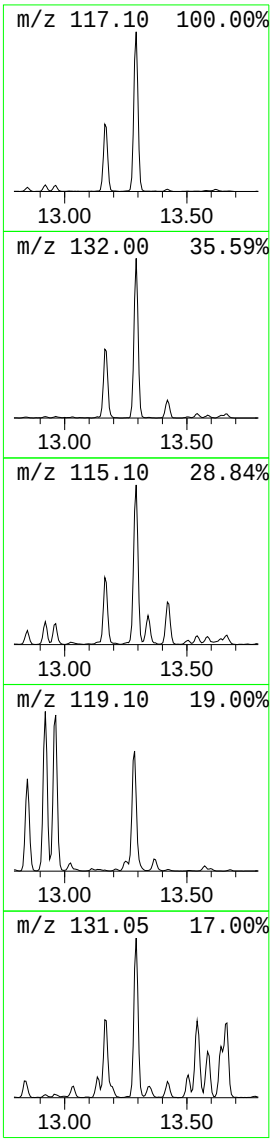
****

Peak Number 10 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	163.11 ug/l	2153460	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	91
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044049.D
Acq On : 27 Nov 2024 18:29
Operator : JC/MD
Sample : P5021-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.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
Butane	1.374	103.5	ug/l	535706	1	5.550	258805	50.0
Butane, 2-methyl-	1.721	255.2	ug/l	1321030	1	5.550	258805	50.0
Pentane	1.935	155.4	ug/l	804258	1	5.550	258805	50.0
Cyclopentane	2.855	111.4	ug/l	576491	1	5.550	258805	50.0
Cyclopentane, m...	4.294	150.5	ug/l	778916	1	5.550	258805	50.0
Benzene, 1-ethy...	11.610	412.7	ug/l	5448690	4	12.018	660141	50.0
Benzene, 1,2,3-...	12.085	492.3	ug/l	6499090	4	12.018	660141	50.0
Indane	12.244	523.2	ug/l	6907590	4	12.018	660141	50.0
Benzene, 4-ethy...	12.610	98.5	ug/l	1300130	4	12.018	660141	50.0
1-Phenyl-1-butene	13.292	163.1	ug/l	2153460	4	12.018	660141	50.0