LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

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\82X061824W.M
Title : SW846 8260

Signal : TIC: VX042328.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	41	rVB	22398	23492	3.12%	0.406%
2	1.599	76	84	86	rBV5	4298	9605	1.27%	0.166%
3	5.385	693	705	718	rBV	76876	241575	32.04%	4.179%
4	5.538	720	730	747	rVB	117995	345760	45.86%	5.982%
5	5.952	788	798	816	rBV	82507	234831	31.14%	4.063%
6	6.598	896	904	911	rBV4	3264	8106	1.08%	0.140%
7	6.757	920	930	941	rBV	182783	447294	59.32%	7.739%
8	7.367	1019	1030	1037	rBV2	6504	15095	2.00%	0.261%
9	8.269	1170	1178	1182	rBV4	4475	8394	1.11%	0.145%
10	8.433	1198	1205	1214	rBV	3757	7559	1.00%	0.131%
11	8.647	1234	1240	1248	rVV	364932	587967	77.98%	10.172%
12	8.720	1248	1252	1257	rVB	29406	46110	6.12%	0.798%
13	8.909	1277	1283	1289	rBV	16447	24292	3.22%	0.420%
14	9.903	1442	1446	1452	rVB2	11039	15827	2.10%	0.274%
15	10.006	1457	1463	1466	rBV2	7266	10437	1.38%	0.181%
16	10.055	1466	1471	1488	rVV	366368	510646	67.72%	8.835%
17	10.195	1488	1494	1502	rVV	24728	35284	4.68%	0.610%
18	10.299	1502	1511	1517	rVV	110890	165030	21.89%	2.855%
19	10.360	1517	1521	1530	rVB	42223	55526	7.36%	0.961%
20	10.586	1551	1558	1562	rBV6	4623	8323	1.10%	0.144%
21	10.640	1562	1567	1576	rVV	48101	71972	9.55%	1.245%
22	10.781	1586	1590	1594	rVB2	7276	9538	1.26%	0.165%
23	10.854	1594	1602	1606	rBV6	8019	13823	1.83%	0.239%
24	11.079	1634	1639	1650	rBV	311103	433901	57.55%	7.507%
25	11.305	1672	1676	1681	rBV	7065	10660	1.41%	0.184%
26	11.378	1684	1688	1695	rVV	28221	52706	6.99%	0.912%
27	11.451	1695	1700	1702	rVV	26881	40795	5.41%	0.706%
28	11.476	1702	1704	1715	rVB	57021	65698	8.71%	1.137%
29	11.616	1722	1727	1733	rBV	8850	14981	1.99%	0.259%
30	11.750	1746	1749	1758	rVB	51837	69606	9.23%	1.204%
31	12.024	1788	1794	1800	rVV	361325	467495	62.00%	8.088%
32	12.085	1800	1804	1811	rVB2	23548	42409	5.62%	0.734%
33	12.317	1838	1842	1850	rVB4	14466	24438	3.24%	0.423%
34	12.421	1853	1859	1864	rBV2	51089	68608	9.10%	1.187%
35	12.469	1864	1867	1874	rVB4	5311	10108	1.34%	0.175%
36	12.719	1900	1908	1913	rBV7	4647	9320	1.24%	0.161%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

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\82X061824W.M
Title : SW846 8260

37	12.817	1918	1924	1927	rBV5	6966	12246	1.62%	0.212%
38	12.890	1932	1936	1938	rVV3	5965	8836	1.17%	0.153%
39	12.920	1938	1941	1945	rVV	10886	16680	2.21%	0.289%
40	12.969	1945	1949	1956	rVV4	12598	24911	3.30%	0.431%
41	13.268	1994	1998	2000	rBV	20851	26213	3.48%	0.454%
42	13.292	2000	2002	2008	rVB2	15350	20030	2.66%	0.347%
43	13.426	2019	2024	2029	rVB8	8015	15429	2.05%	0.267%
44	13.774	2076	2081	2089	rVV	602331	754017	100.00%	13.045%
45	13.841	2089	2092	2095	rVV5	5152	8894	1.18%	0.154%
46	13.872	2095	2097	2100	rVB	7972	8479	1.12%	0.147%
47	14.036	2118	2124	2127	rBV2	13079	17563	2.33%	0.304%
48	14.219	2148	2154	2159	rVB6	8355	12777	1.69%	0.221%
49	14.432	2183	2189	2193	rVB7	4282	8061	1.07%	0.139%
50	14.640	2215	2223	2233	rVV	121426	167269	22.18%	2.894%
51	14.780	2239	2246	2253	rVB2	87414	137662	18.26%	2.382%
52	15.213	2313	2317	2321	rVB	20161	27742	3.68%	0.480%
53	15.377	2340	2344	2347	rBV3	11358	16890	2.24%	0.292%
54	15.414	2347	2350	2354	rVB5	7177	11089	1.47%	0.192%
55	15.481	2355	2361	2370	rBV2	35530	70309	9.32%	1.216%
56	15.615	2378	2383	2386	rBV	37762	60464	8.02%	1.046%
57	15.652	2386	2389	2399	rVB	23620	38180	5.06%	0.661%
58	15.835	2412	2419	2424	rBV2	8842	20070	2.66%	0.347%
59	15.920	2429	2433	2439	rVB7	7179	13231	1.75%	0.229%
60	15.987	2439	2444	2449	rBV3	7344	13947	1.85%	0.241%
61	16.091	2456	2461	2470	rBV3	12644	27411	3.64%	0.474%
62	16.377	2501	2508	2512	rVB3	11385	23246	3.08%	0.402%
63	16.603	2541	2545	2550	rVB5	6788	11207	1.49%	0.194%

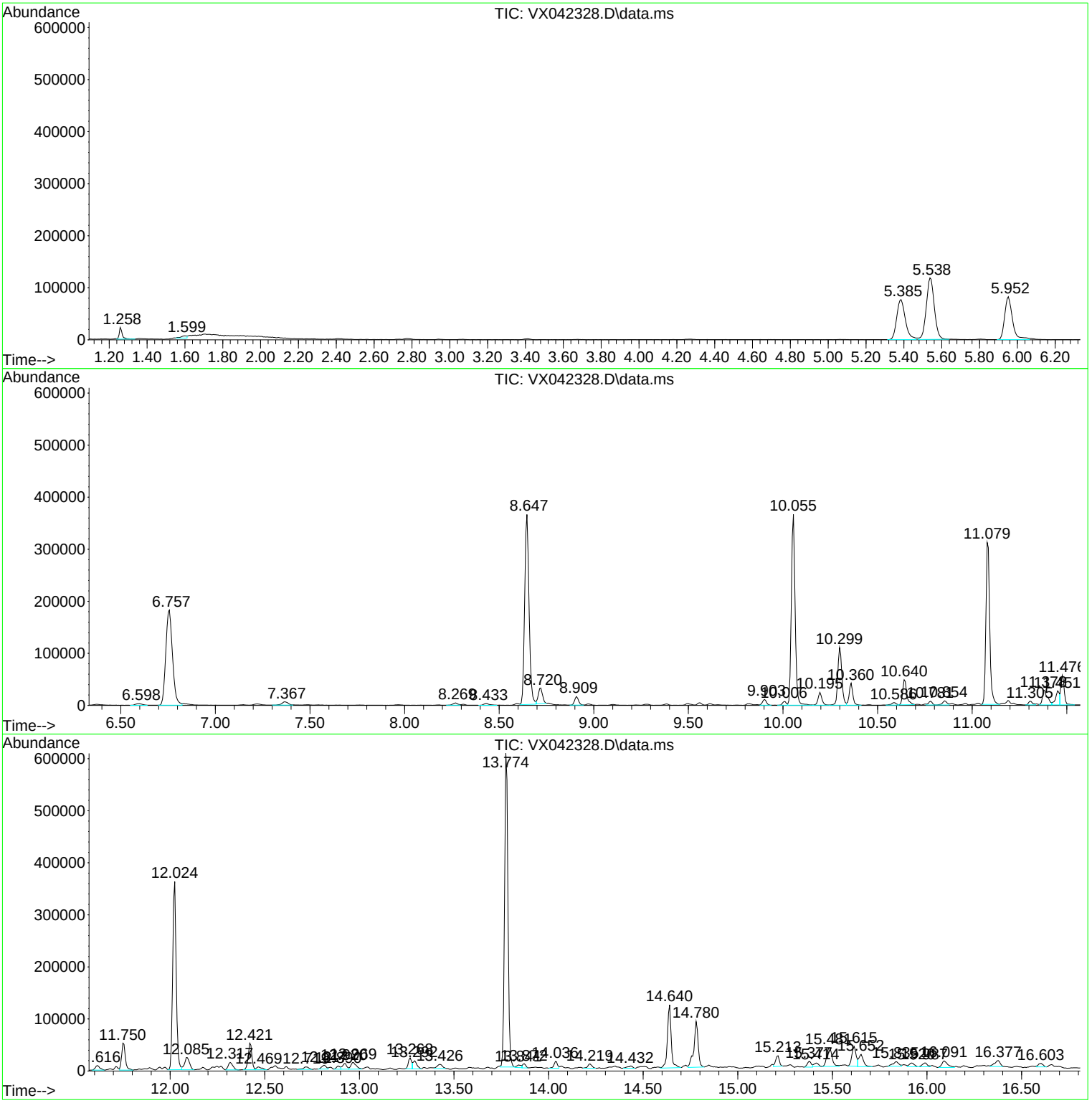
Sum of corrected areas: 5780064

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

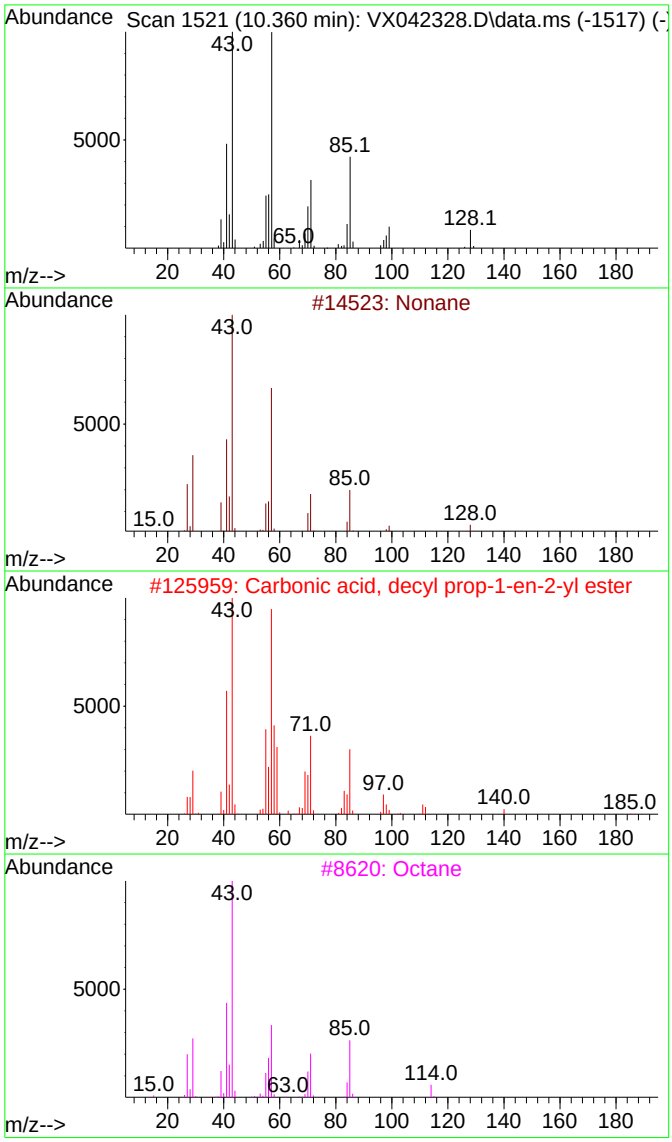
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

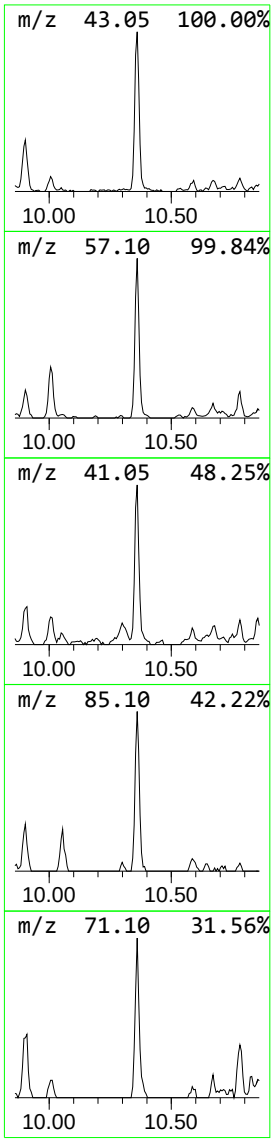
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Nonane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	5.44 ug/l	55526	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	95
2	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	72
3	Octane	114	C8H18	000111-65-9	64
4	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	59
5	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

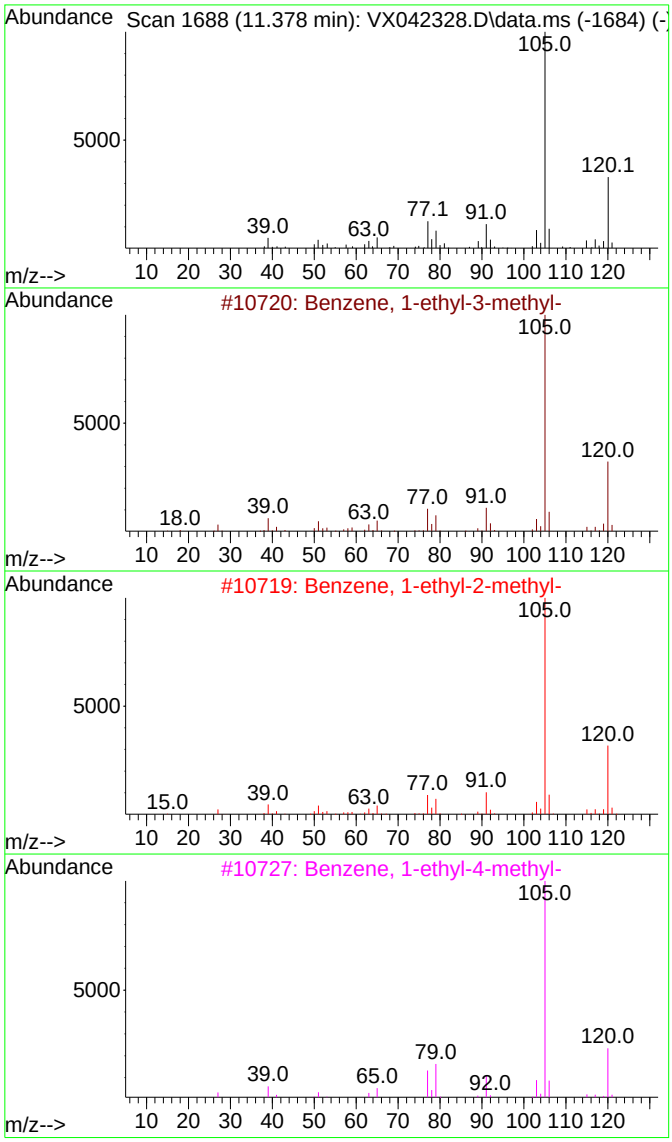
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

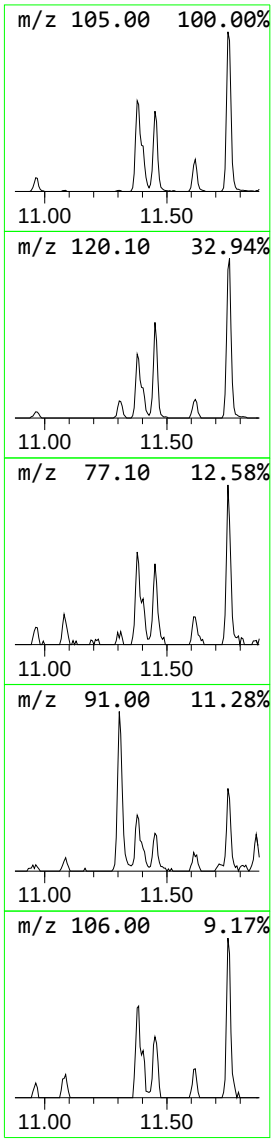
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.64 ug/l	52706	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

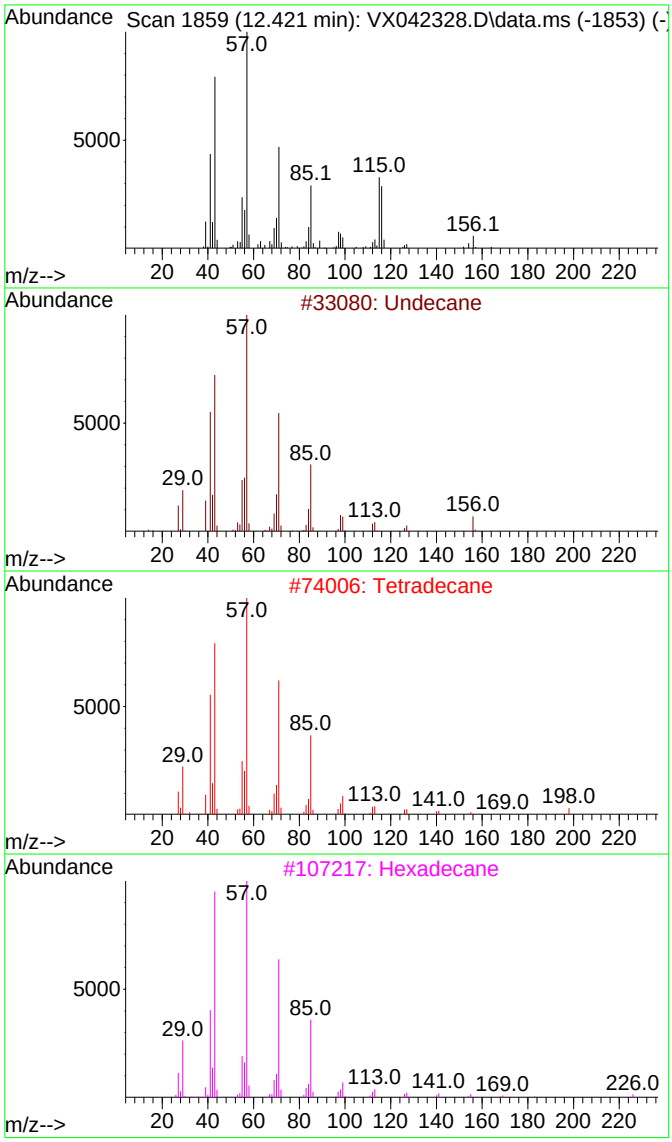
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

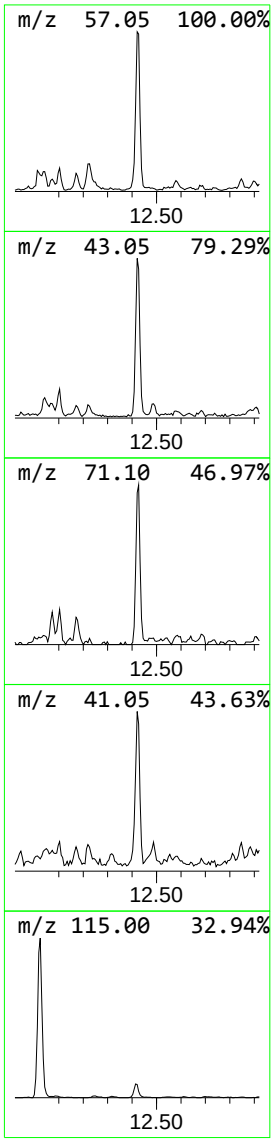
****

Peak Number 3 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	7.34 ug/l	68608	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Tetradecane	198	C14H30	000629-59-4	52
3	Hexadecane	226	C16H34	000544-76-3	52
4	Tridecane	184	C13H28	000629-50-5	50
5	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

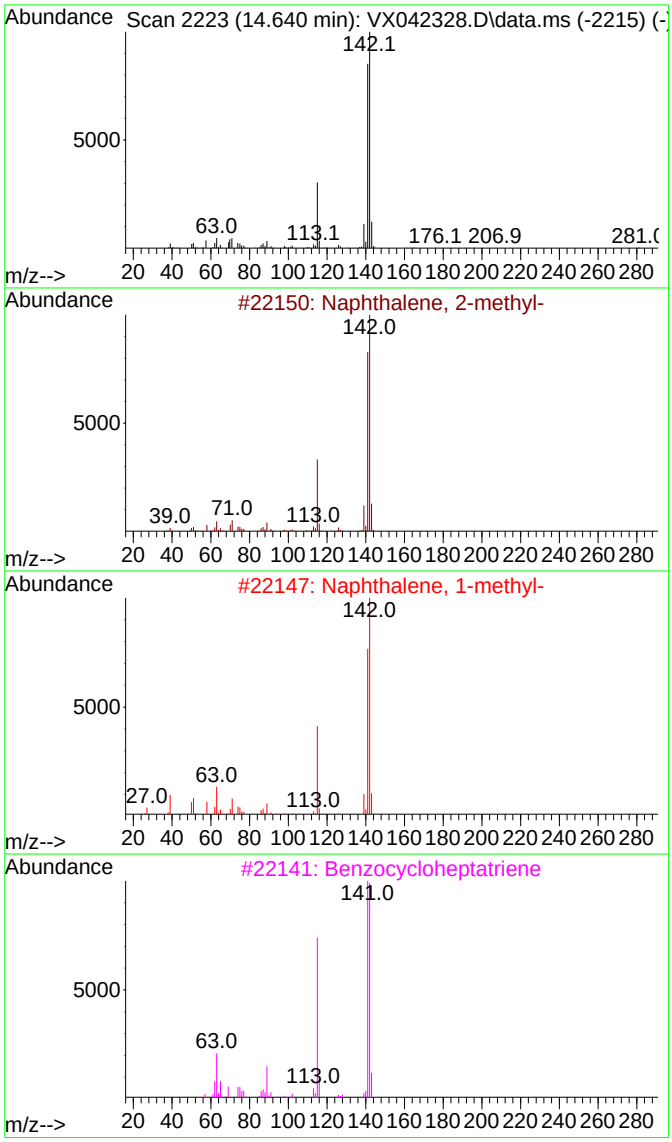
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

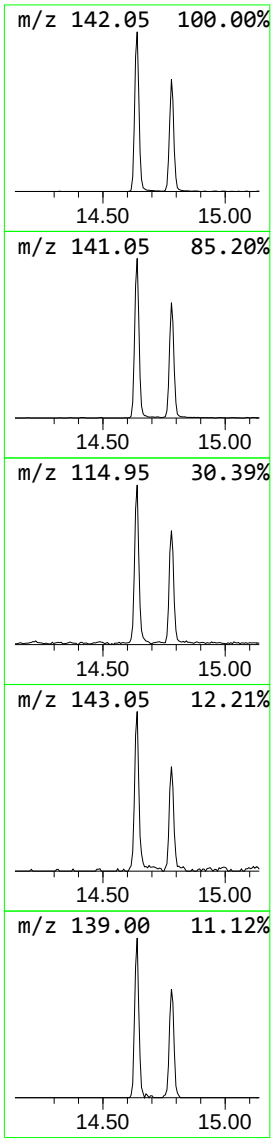
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	17.89 ug/l	167269	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

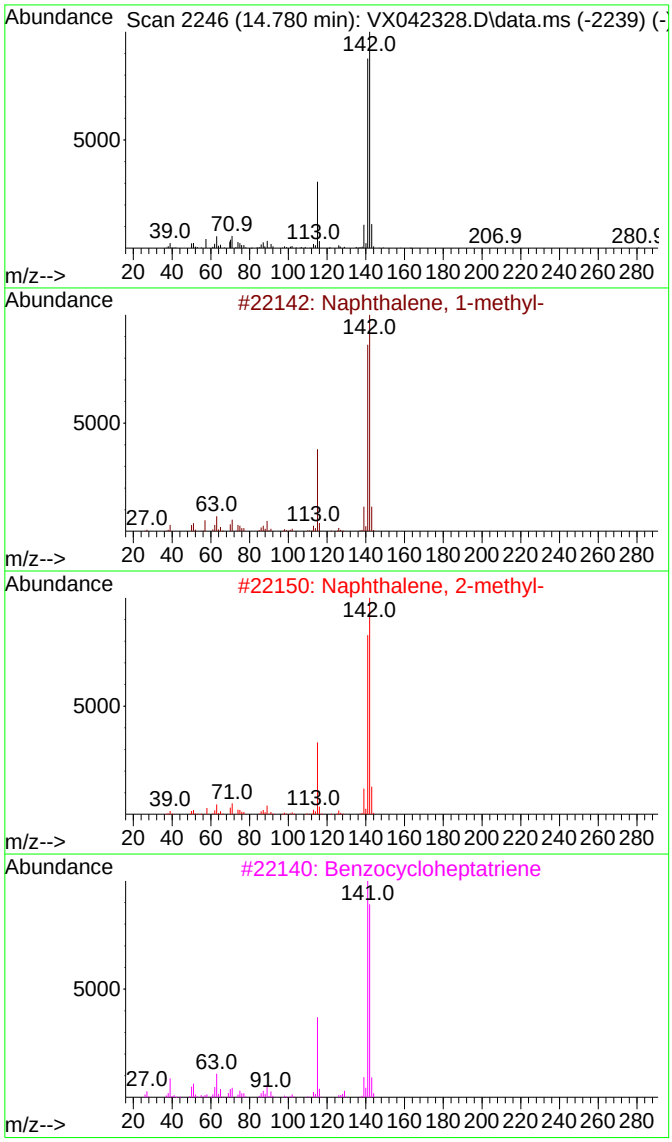
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

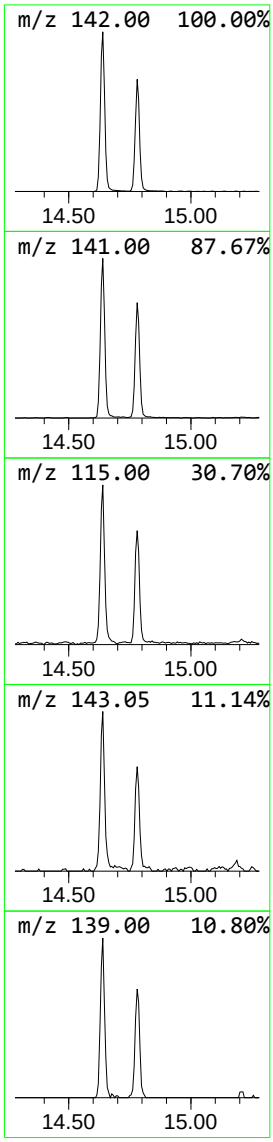
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	14.72 ug/l	137662	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

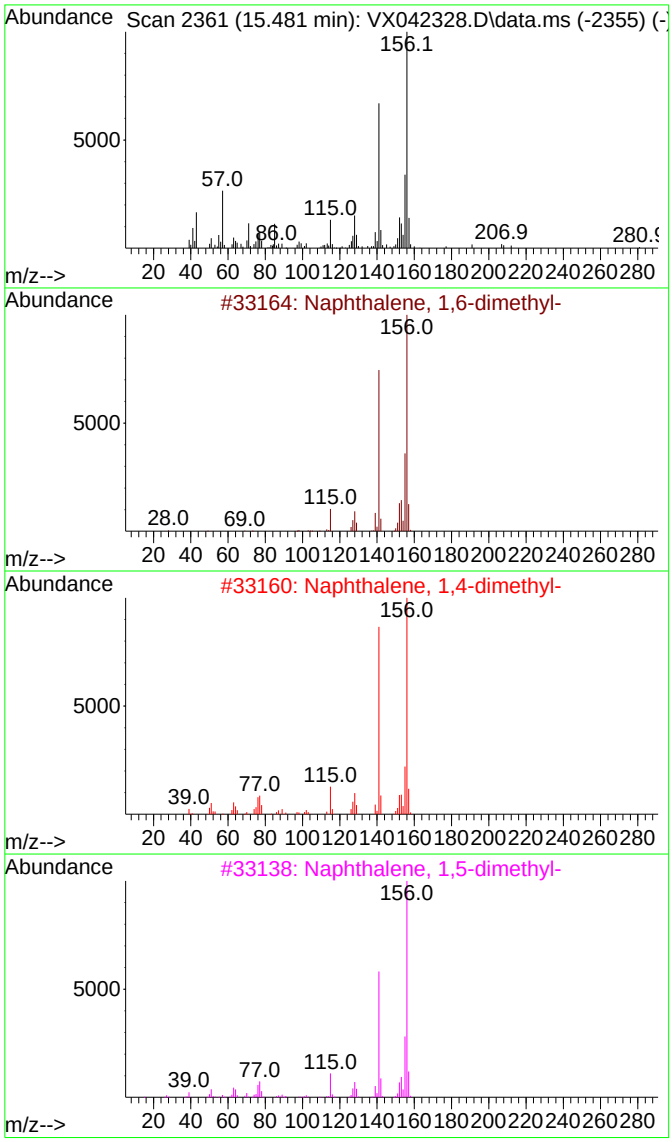
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

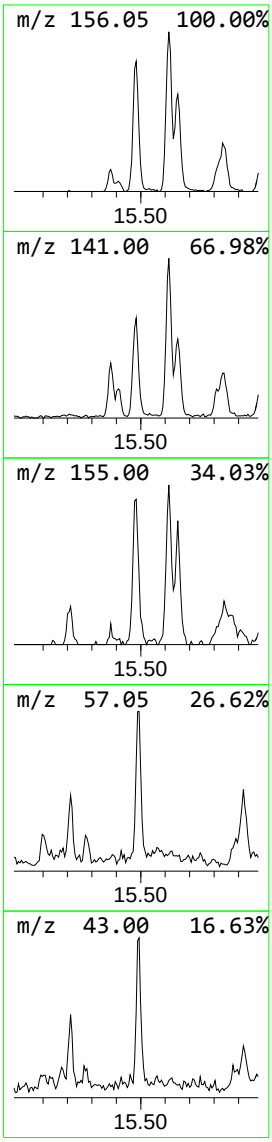
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	7.52 ug/l	70309	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	96
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

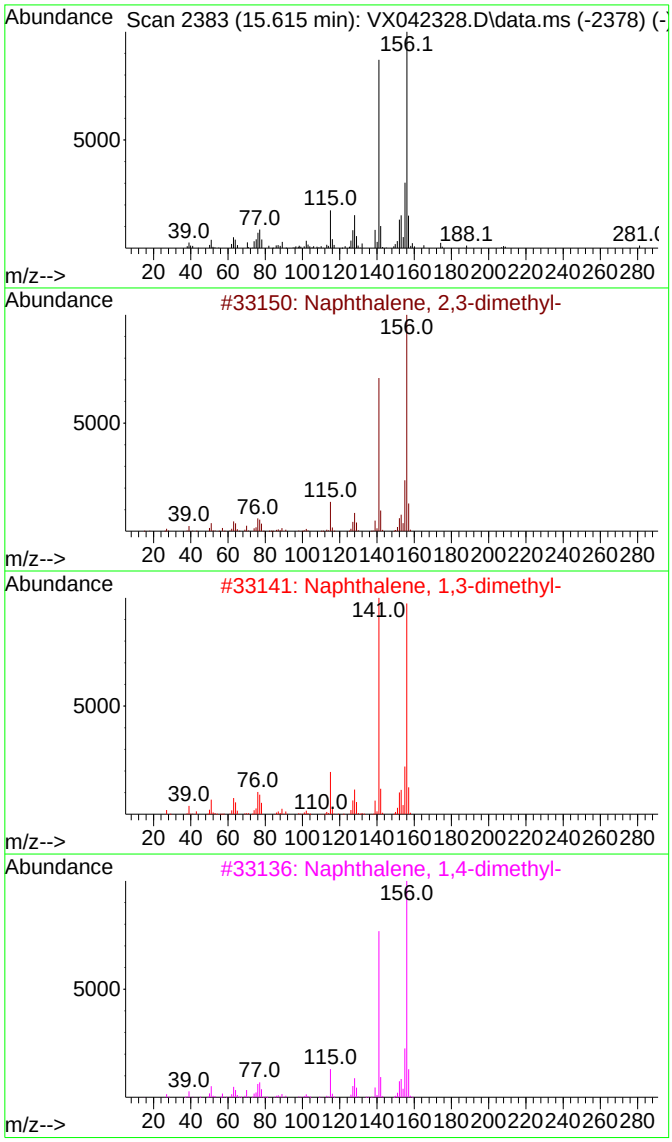
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

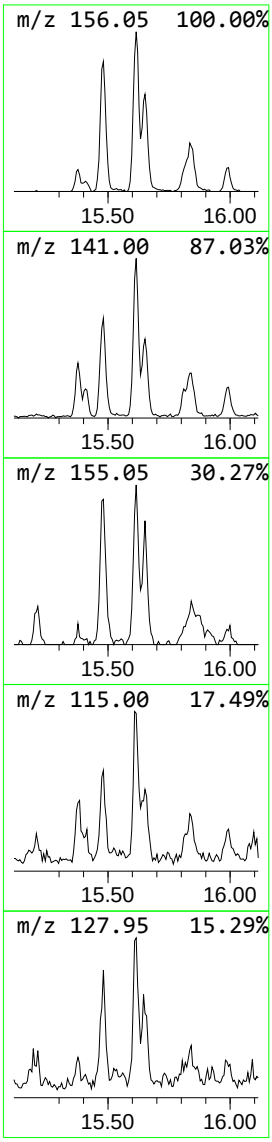
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	6.47 ug/l	60464	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
Data File : VX042328.D
Acq On : 15 Jul 2024 16:13
Operator : JC/MD
Sample : P3224-33
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
356STEVEN-18

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.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
Nonane	10.360	5.4	ug/l	55526	3	10.055	510646	50.0
Benzene, 1-ethy...	11.378	5.6	ug/l	52706	4	12.024	467495	50.0
Undecane	12.421	7.3	ug/l	68608	4	12.024	467495	50.0
Naphthalene, 2-...	14.640	17.9	ug/l	167269	4	12.024	467495	50.0
Naphthalene, 1-...	14.780	14.7	ug/l	137662	4	12.024	467495	50.0
Naphthalene, 1,...	15.481	7.5	ug/l	70309	4	12.024	467495	50.0
Naphthalene, 2,...	15.615	6.5	ug/l	60464	4	12.024	467495	50.0