LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	694	705	718	rBV	73423	210987	33.56%	4.336%
2	5.549	721	732	750	rVB	125260	355179	56.49%	7.300%
3	5.958	788	799	816	rBV2	81310	216784	34.48%	4.455%
4	6.763	921	931	948	rBV	198504	464376	73.85%	9.544%
5	8.646	1234	1240	1255	rBV	391326	628771	100.00%	12.922%
6	10.055	1465	1471	1486	rBV	406738	536652	85.35%	11.029%
7	11.079	1634	1639	1650	rBV	322049	417410	66.39%	8.579%
8	11.481	1700	1705	1709	rVB	12673	16390	2.61%	0.337%
9	11.719	1740	1744	1747	rBV2	7299	8942	1.42%	0.184%
10	11.750	1747	1749	1759	rVB5	3524	8658	1.38%	0.178%
11	11.890	1766	1772	1776	rBV7	4710	7242	1.15%	0.149%
12	11.939	1776	1780	1784	rBV4	8804	14029	2.23%	0.288%
13	12.024	1789	1794	1800	rBV	412059	508518	80.87%	10.451%
14	12.103	1804	1807	1812	rVB3	9623	10358	1.65%	0.213%
15	12.176	1816	1819	1825	rVB	11730	16740	2.66%	0.344%
16	12.262	1825	1833	1837	rBV7	5589	14750	2.35%	0.303%
17	12.317	1837	1842	1848	rBV9	12346	26117	4.15%	0.537%
18	12.384	1848	1853	1854	rBV3	6503	9299	1.48%	0.191%
19	12.426	1855	1860	1864	rVB	114698	132979	21.15%	2.733%
20	12.469	1864	1867	1874	rVB4	16878	30322	4.82%	0.623%
21	12.554	1874	1881	1884	rBV2	18124	37080	5.90%	0.762%
22	12.640	1891	1895	1899	rVB4	4937	7390	1.18%	0.152%
23	12.682	1899	1902	1906	rBV3	12403	18099	2.88%	0.372%
24	12.719	1906	1908	1912	rVV5	6006	10558	1.68%	0.217%
25	12.762	1912	1915	1917	rVV3	10885	14969	2.38%	0.308%
26	12.816	1920	1924	1930	rVB2	24864	35785	5.69%	0.735%
27	12.890	1931	1936	1943	rVV5	36824	69520	11.06%	1.429%
28	12.944	1943	1945	1946	rVV	8639	7696	1.22%	0.158%
29	12.981	1947	1951	1957	rVV6	23303	39338	6.26%	0.808%
30	13.042	1957	1961	1965	rVB2	15499	18180	2.89%	0.374%
31	13.152	1975	1979	1982	rBV5	4950	9152	1.46%	0.188%
32	13.268	1994	1998	2001	rBV	48186	63505	10.10%	1.305%
33	13.292	2001	2002	2008	rVB2	27552	30357	4.83%	0.624%
34	13.347	2008	2011	2015	rBV6	7549	8606	1.37%	0.177%
35	13.383	2015	2017	2019	rBV2	6495	7427	1.18%	0.153%
36	13.414	2019	2022	2032	rVB8	17387	41577	6.61%	0.854%

LSC Area Percent Report

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Data File : VX032574.D
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Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

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\82X102622W.M
Title : SW846 8260

37	13.499	2032	2036	2041	rBV7	5730	9204	1.46%	0.189%
38	13.676	2061	2065	2072	rBV9	5679	18215	2.90%	0.374%
39	13.737	2072	2075	2078	rVV	7347	10087	1.60%	0.207%
40	13.798	2082	2085	2089	rVB5	6876	8374	1.33%	0.172%
41	13.841	2089	2092	2095	rBV5	5210	6915	1.10%	0.142%
42	13.908	2101	2103	2112	rVB8	5426	10049	1.60%	0.207%
43	14.219	2151	2154	2157	rBV5	7554	10738	1.71%	0.221%
44	14.438	2187	2190	2193	rVB2	9243	11163	1.78%	0.229%
45	14.487	2193	2198	2206	rBV6	8718	19497	3.10%	0.401%
46	14.554	2206	2209	2211	rBV4	7481	8702	1.38%	0.179%
47	14.615	2216	2219	2222	rVV3	19444	26273	4.18%	0.540%
48	14.670	2225	2228	2232	rVB3	17462	21888	3.48%	0.450%
49	14.755	2239	2242	2244	rBV4	9884	8448	1.34%	0.174%
50	14.792	2244	2248	2251	rBV4	16227	17537	2.79%	0.360%
51	14.847	2254	2257	2261	rVV4	13976	18414	2.93%	0.378%
52	15.042	2284	2289	2293	rBV4	21018	36803	5.85%	0.756%
53	15.090	2294	2297	2301	rVV6	8306	14363	2.28%	0.295%
54	15.212	2314	2317	2321	rVB4	16179	18832	3.00%	0.387%
55	15.310	2331	2333	2339	rVB7	11701	21543	3.43%	0.443%
56	15.377	2340	2344	2348	rBV3	36103	55573	8.84%	1.142%
57	15.560	2370	2374	2378	rBV2	71351	97521	15.51%	2.004%
58	15.779	2407	2410	2415	rVB2	40854	58736	9.34%	1.207%
59	15.859	2419	2423	2430	rVB7	27132	66487	10.57%	1.366%
60	16.011	2441	2448	2456	rVB6	45064	138355	22.00%	2.843%
61	16.090	2456	2461	2467	rBV8	40691	98289	15.63%	2.020%

Sum of corrected areas: 4865748

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
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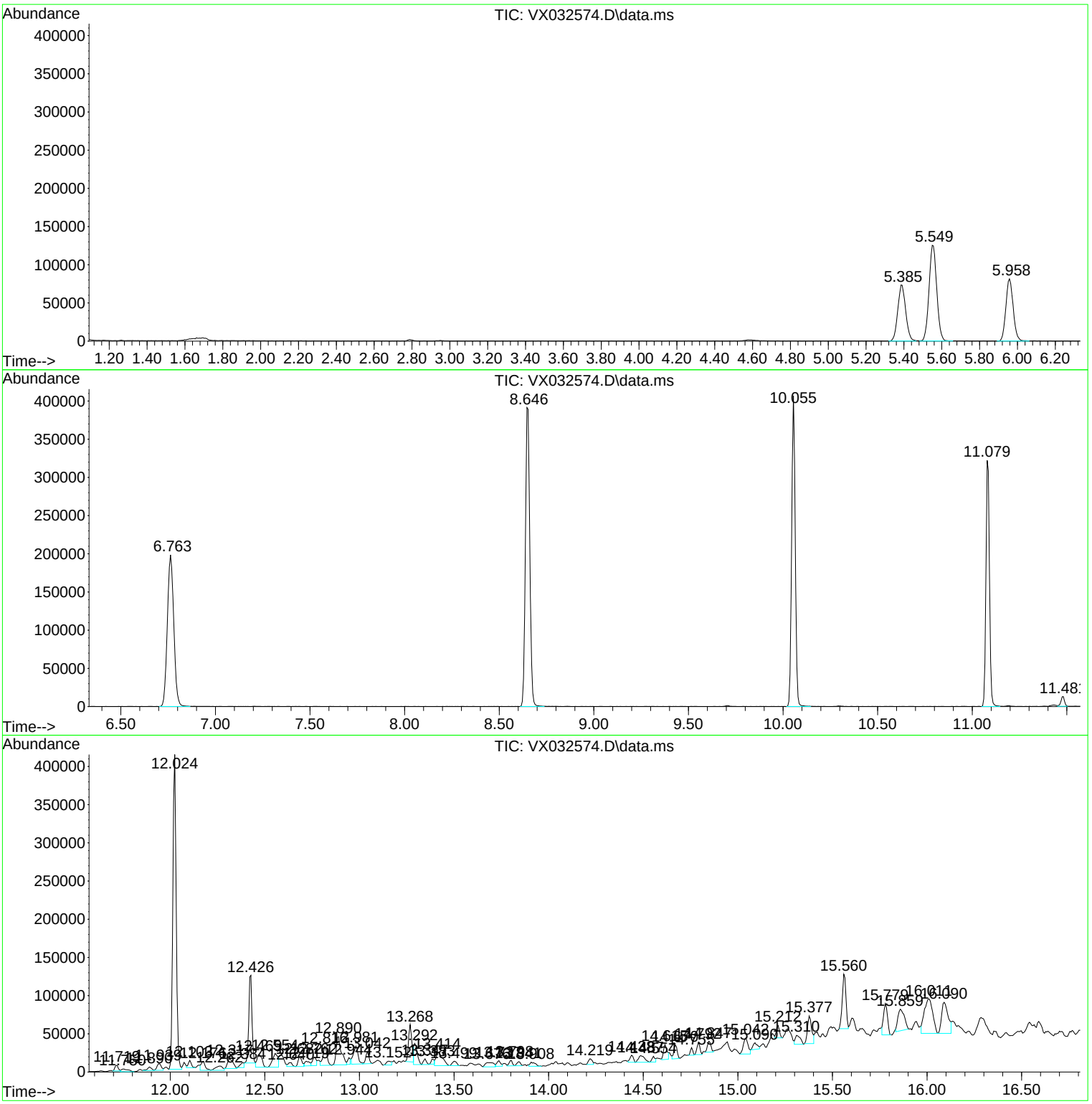
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

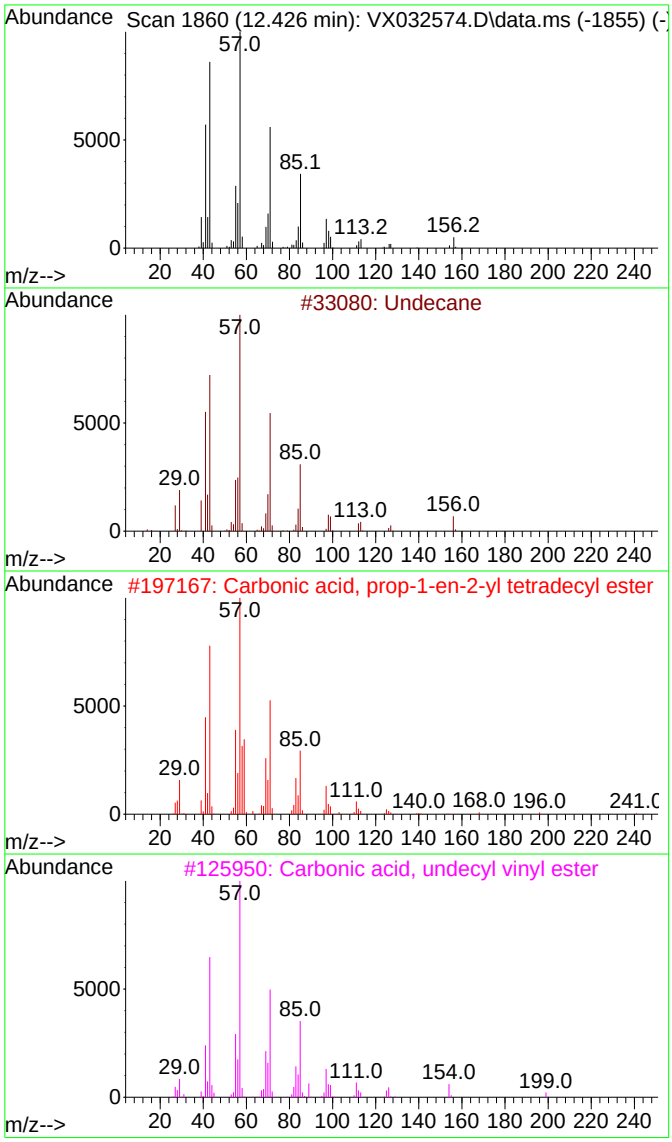
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

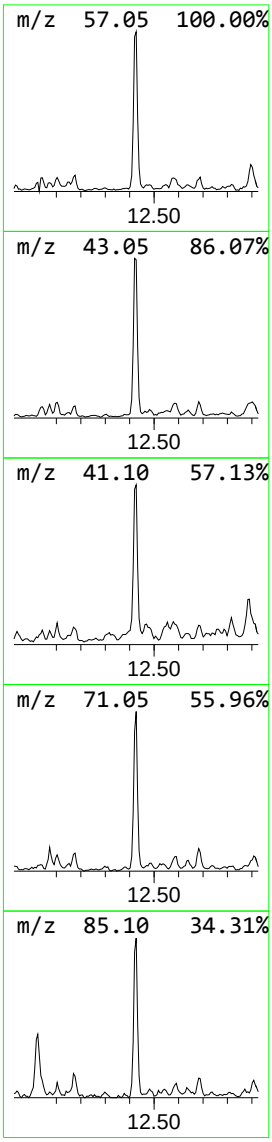
****

Peak Number 1 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.426	13.08 ug/l	132979	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	91
3	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	90
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	86
5	Tetradecane	198	C14H30	000629-59-4	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

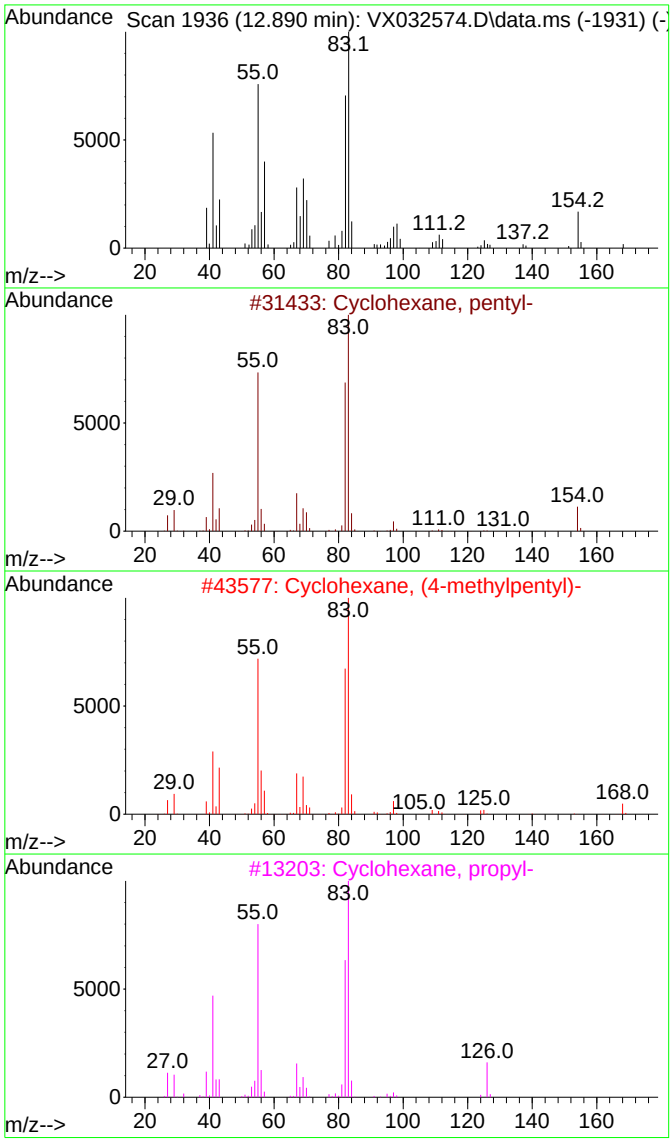
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

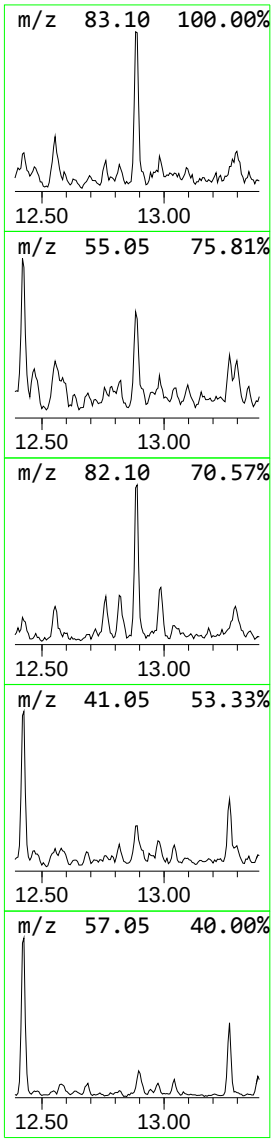
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, pentyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	6.84 ug/l	69520	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	72
2	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	59
3	Cyclohexane, propyl-	126	C9H18	001678-92-8	59
4	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	58
5	3-Cyclohexyl-1-chloropropane	160	C9H17Cl	001124-62-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

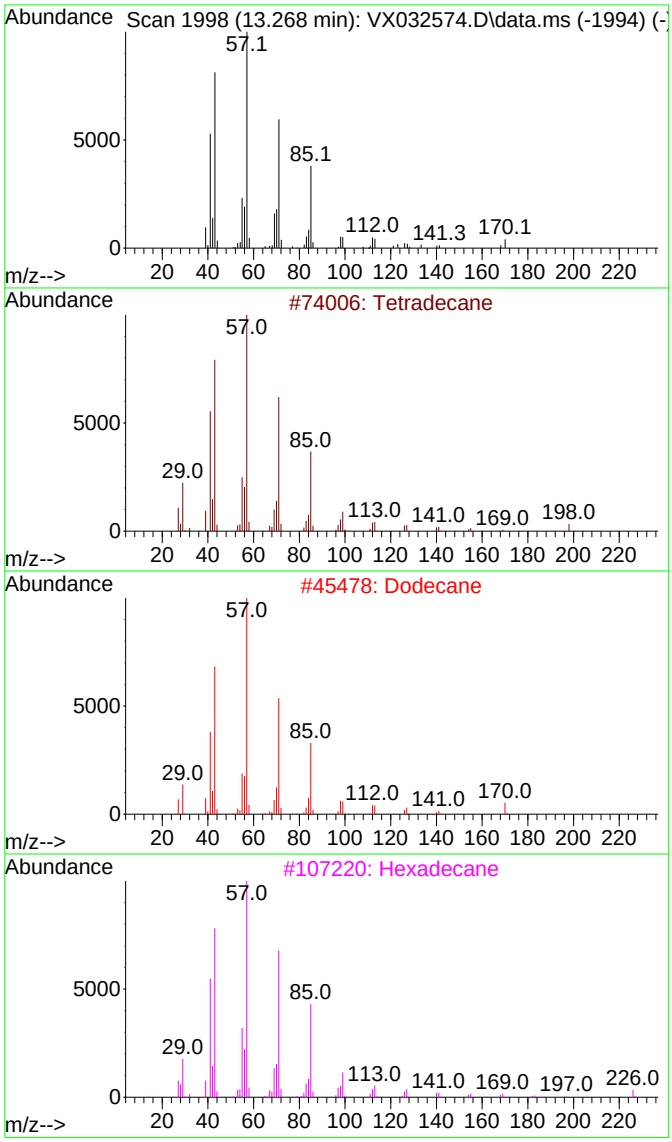
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

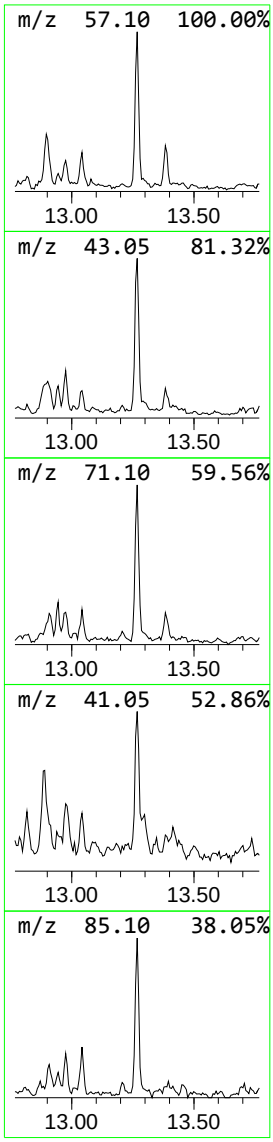
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	6.24 ug/l	63505	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Dodecane	170	C12H26	000112-40-3	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	78
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

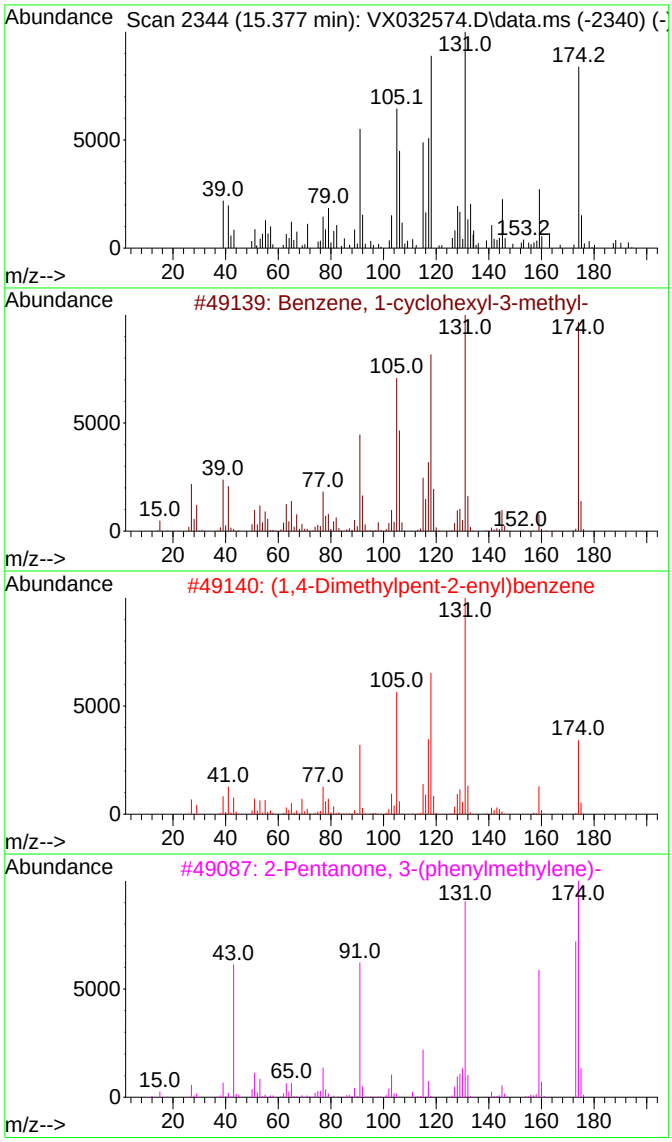
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

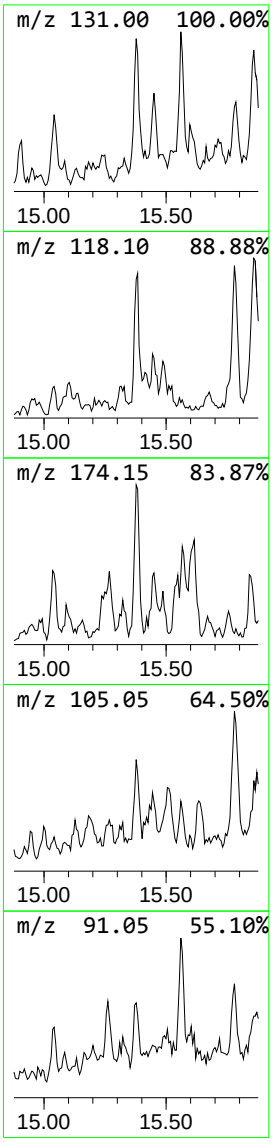
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-cyclohexyl-3-met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	5.46 ug/l	55573	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	94
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	64
3	2-Pentanone, 3-(phenylmethylene)-	174	C12H14O	003437-89-6	55
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	47
5	1H-1,3,2-Benzodiazaborole, 2-but...	174	C10H15BN2	031748-14-8	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

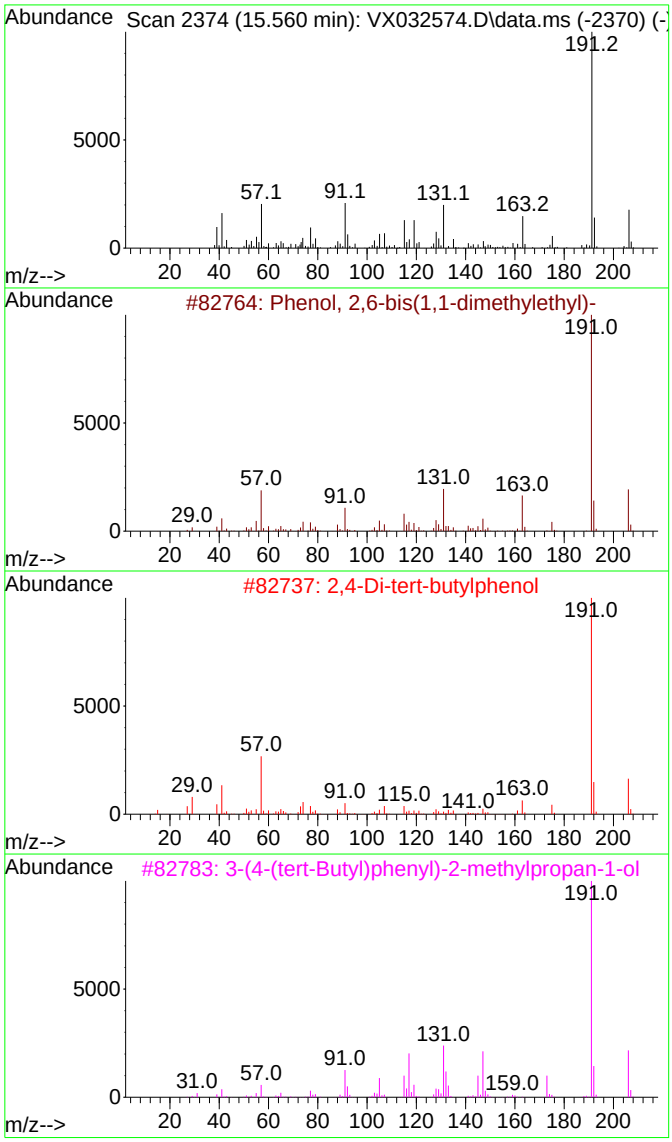
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

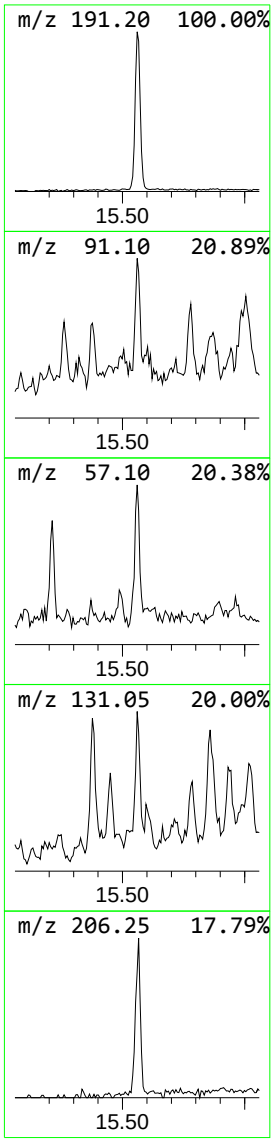
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	9.59 ug/l	97521	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	93
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	76
3	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	72
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	70
5	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

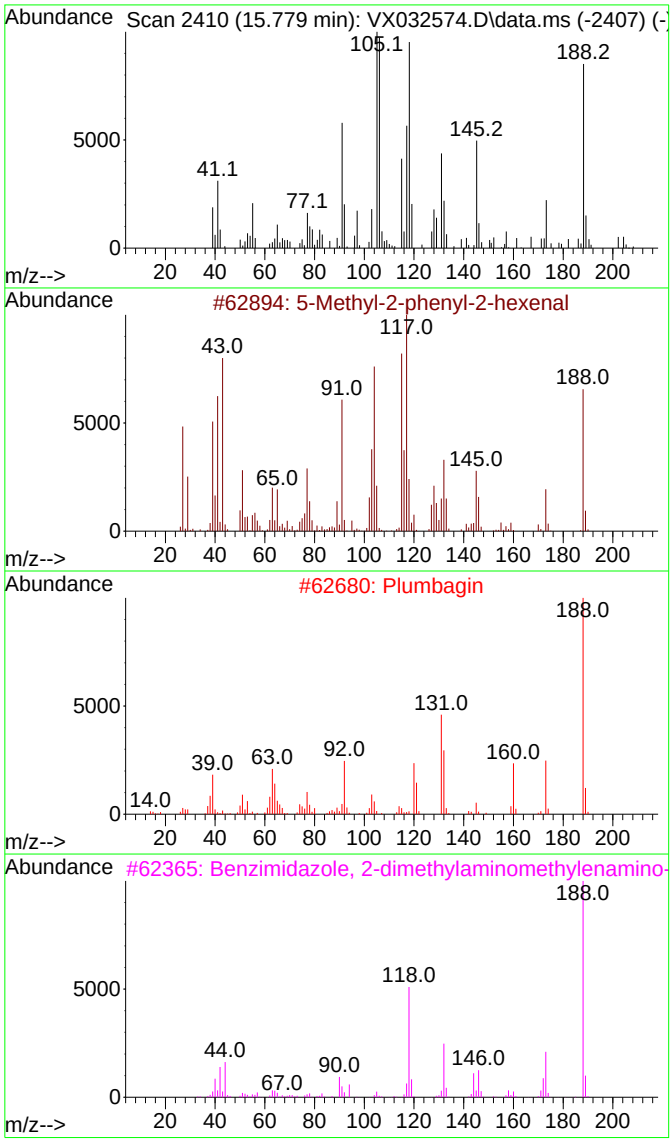
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

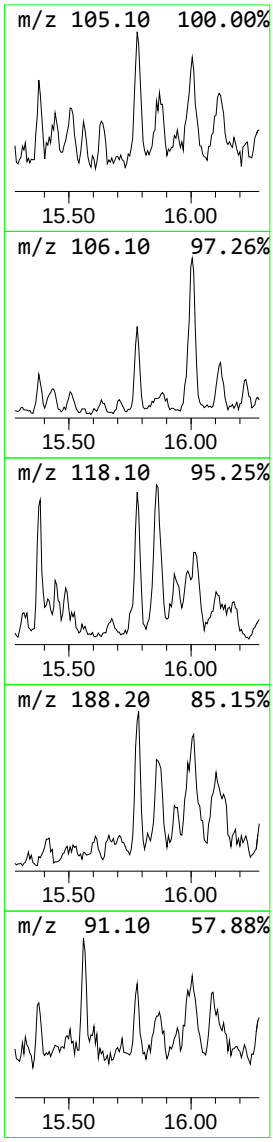
****

Peak Number 6 unknown15.779 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.779	5.78 ug/l	58736	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenyl-2-hexenal	188	C13H16O	021834-92-4	45
2	Plumbagin	188	C11H8O3	000481-42-5	30
3	Benzimidazole, 2-dimethylaminome...	188	C10H12N4	060308-65-8	25
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	22
5	2-Methylinden-3-one carboxylic acid	188	C11H8O3	1000214-94-6	18





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

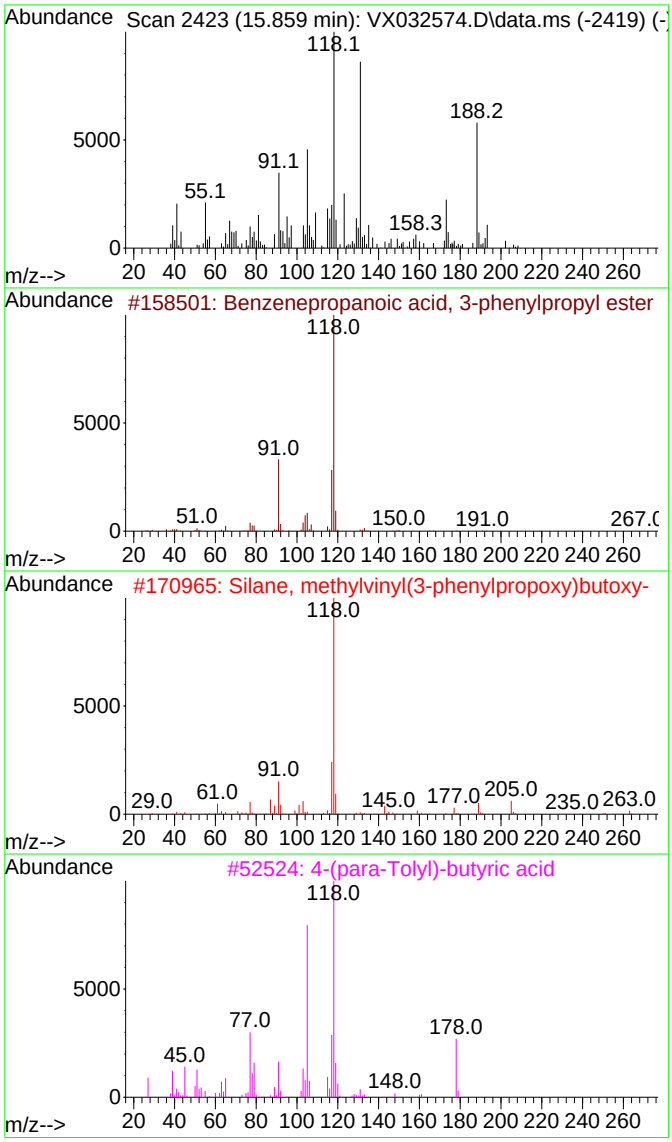
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

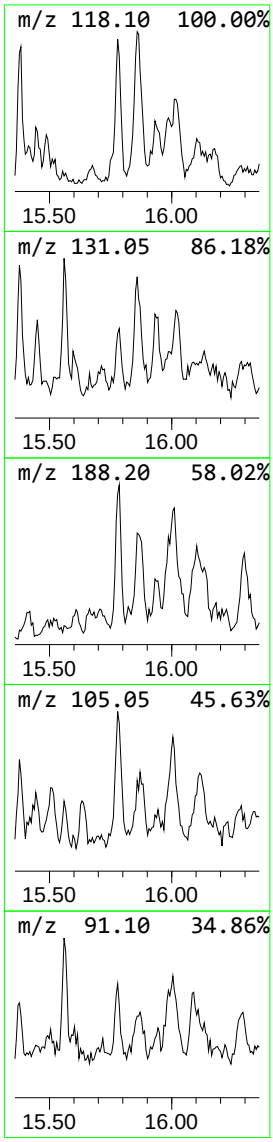
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown15.858 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.858	6.54 ug/l	66487	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 3-phenylp...	268	C18H20O2	060045-27-4	22
2	Silane, methylvinyl(3-phenylprop...	278	C16H26O2Si	1010420-67-6	22
3	4-(para-Tolyl)-butyric acid	178	C11H14O2	004521-22-6	22
4	Succinic acid, cyclohexylmethyl ...	332	C20H28O4	1010389-73-0	22
5	Silane, methylvinyldi(3-phenylpr...	340	C21H28O2Si	1000420-68-1	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

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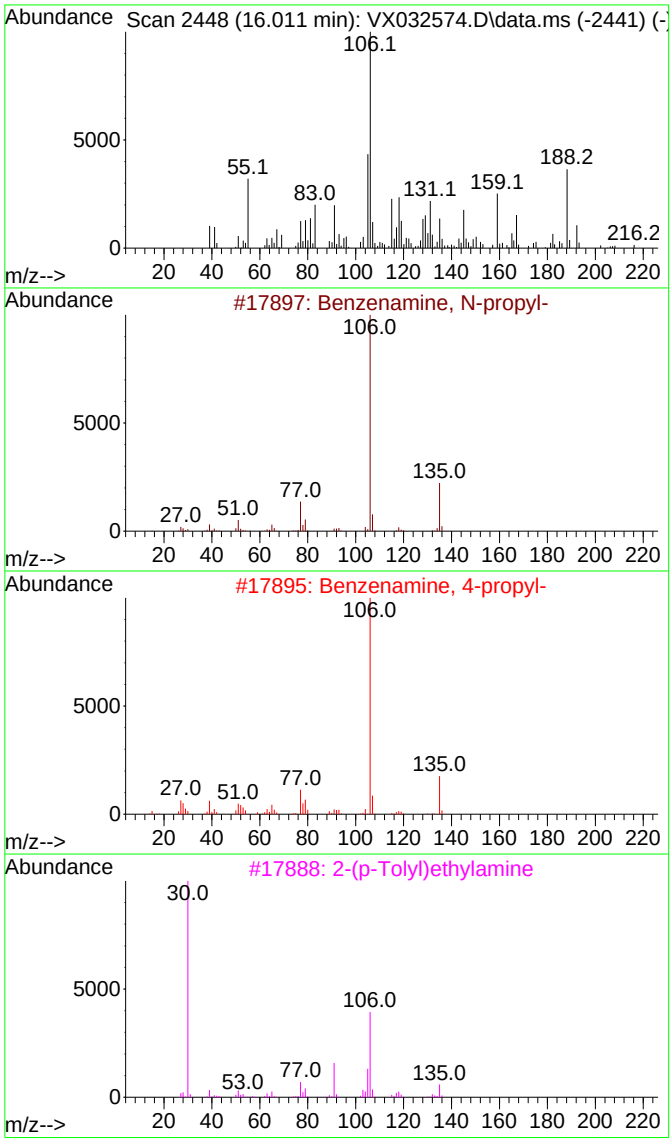
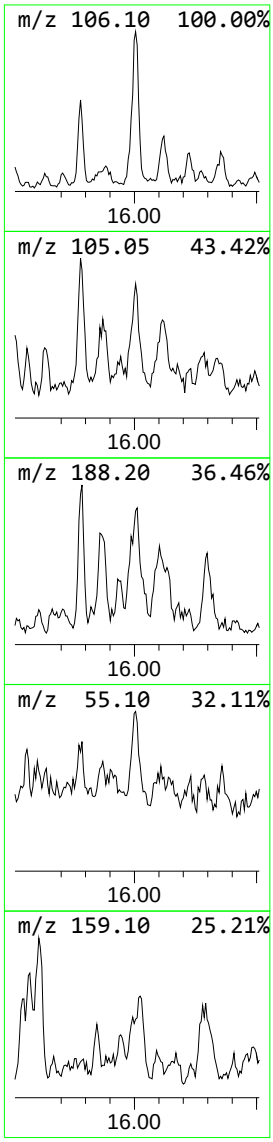
Peak Number 8 unknown16.011 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	13.60 ug/l	138355	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N-propyl-	135	C9H13N	000622-80-0	38
2	Benzenamine, 4-propyl-	135	C9H13N	002696-84-6	38
3	2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	38
4	Benzenamine, 2-propyl-	135	C9H13N	001821-39-2	35
5	Benzenamine, N-butyl-	149	C10H15N	001126-78-9	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

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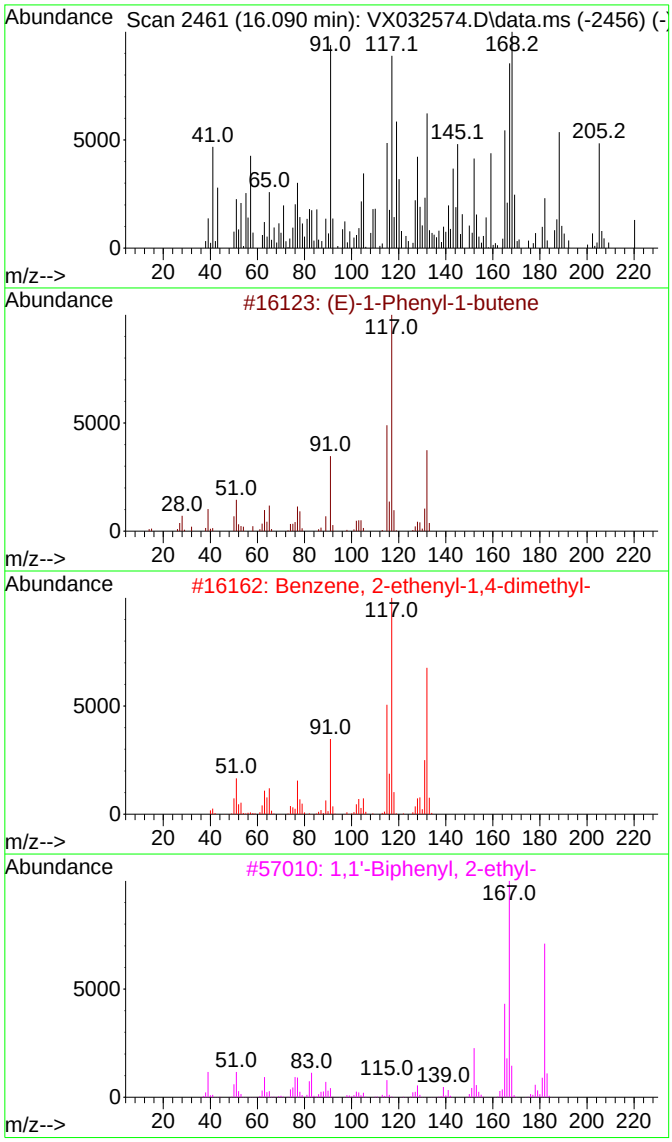
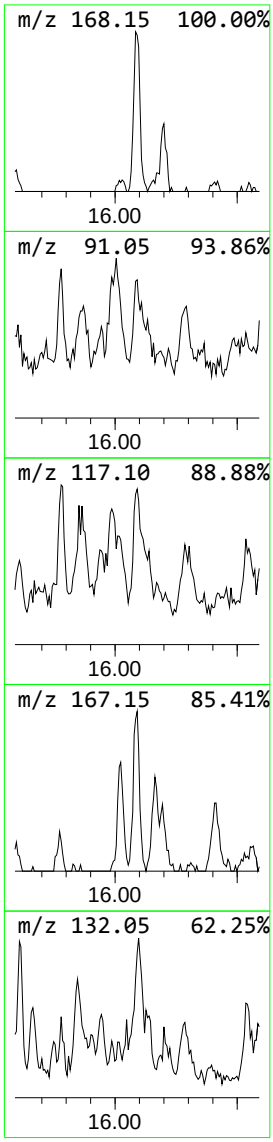
Peak Number 9 unknown16.090 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.090	9.66 ug/l	98289	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	40
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	40
3	1,1'-Biphenyl, 2-ethyl-	182	C14H14	001812-51-7	35
4	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	30
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110422\
Data File : VX032574.D
Acq On : 04 Nov 2022 14:19
Operator : JC/MD
Sample : N5387-03 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
32505

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Undecane	12.426	13.1	ug/l	132979	4	12.024	508518	50.0
Cyclohexane, pe...	12.890	6.8	ug/l	69520	4	12.024	508518	50.0
Tetradecane	13.268	6.2	ug/l	63505	4	12.024	508518	50.0
Benzene, 1-cycl...	15.377	5.5	ug/l	55573	4	12.024	508518	50.0
Phenol, 2,6-bis...	15.560	9.6	ug/l	97521	4	12.024	508518	50.0
unknown15.779	15.779	5.8	ug/l	58736	4	12.024	508518	50.0
unknown15.858	15.858	6.5	ug/l	66487	4	12.024	508518	50.0
unknown16.011	16.011	13.6	ug/l	138355	4	12.024	508518	50.0
unknown16.090	16.090	9.7	ug/l	98289	4	12.024	508518	50.0