LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.693	14	18	23	rBV	101805	137115	2.00%	0.174%
2	4.004	66	71	77	rVB	215485	291851	4.25%	0.371%
3	4.299	116	121	126	rVB	151240	205321	2.99%	0.261%
4	4.822	203	210	214	rBV	384598	538423	7.85%	0.685%
5	4.863	214	217	222	rVB	166277	226762	3.30%	0.288%
6	5.481	318	322	328	rBV	73015	109187	1.59%	0.139%
7	5.546	328	333	337	rVV	120485	180928	2.64%	0.230%
8	5.593	337	341	345	rVV	67745	96281	1.40%	0.122%
9	5.646	345	350	358	rVB	115186	204962	2.99%	0.261%
10	5.946	395	401	407	rVB	64990	97939	1.43%	0.125%
11	6.587	504	510	513	rBV2	56297	91599	1.33%	0.116%
12	7.004	574	581	586	rBV	135222	205175	2.99%	0.261%
13	7.687	690	697	704	rBV	353837	580860	8.46%	0.739%
14	7.869	721	728	737	rBV	1251611	2006542	29.24%	2.551%
15	8.087	758	765	772	rBV	1362075	2194987	31.99%	2.791%
16	8.569	840	847	856	rBV	1368268	2278170	33.20%	2.897%
17	9.263	953	965	977	rBV	998594	1704862	24.84%	2.168%
18	9.751	1041	1048	1056	rBV	1508640	2585740	37.68%	3.288%
19	10.145	1104	1115	1124	rBV5	32589	85695	1.25%	0.109%
20	10.316	1137	1144	1149	rBV6	34318	87374	1.27%	0.111%
21	10.481	1165	1172	1187	rVB	1124708	1948480	28.40%	2.478%
22	10.875	1232	1239	1246	rVB5	28956	77963	1.14%	0.099%
23	11.022	1257	1264	1285	rVB	1772130	3158772	46.03%	4.017%
24	11.257	1298	1304	1312	rBV3	63926	132844	1.94%	0.169%
25	11.416	1324	1331	1342	rBV	1730523	3052685	44.49%	3.882%
26	11.539	1345	1352	1357	rBV	156596	284250	4.14%	0.361%
27	11.604	1357	1363	1370	rBV	368982	694760	10.12%	0.883%
28	11.710	1377	1381	1386	rBV	90362	130817	1.91%	0.166%
29	11.822	1397	1400	1412	rVB4	54745	124510	1.81%	0.158%
30	12.080	1435	1444	1452	rBV9	22963	85541	1.25%	0.109%
31	12.257	1468	1474	1483	rBV	791673	1286765	18.75%	1.636%
32	12.510	1513	1517	1524	rVB2	57676	101117	1.47%	0.129%
33	12.957	1587	1593	1598	rBV6	48191	128685	1.88%	0.164%
34	13.239	1637	1641	1646	rBV3	100840	145886	2.13%	0.186%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Title : SVOA CALIBRATION

35	13.539	1687	1692	1699	rVB7	39008	86228	1.26%	0.110%
36	13.727	1720	1724	1730	rVB3	55223	91008	1.33%	0.116%
37	14.004	1767	1771	1777	rBV	116343	162540	2.37%	0.207%
38	14.145	1792	1795	1801	rVB6	50926	82236	1.20%	0.105%
39	14.504	1853	1856	1859	rBV4	54317	80520	1.17%	0.102%
40	14.557	1859	1865	1874	rVB	2910987	3964070	57.77%	5.041%
41	14.757	1895	1899	1907	rVB8	58261	120157	1.75%	0.153%
42	14.868	1912	1918	1924	rBV	3406100	5147601	75.02%	6.545%
43	15.168	1961	1969	1977	rVB2	2243539	3527839	51.41%	4.486%
44	15.316	1990	1994	2000	rVB3	266986	400324	5.83%	0.509%
45	15.639	2046	2049	2053	rVB4	65812	84424	1.23%	0.107%
46	15.698	2056	2059	2064	rVB	101755	141196	2.06%	0.180%
47	15.868	2085	2088	2092	rBV	97589	133519	1.95%	0.170%
48	16.145	2129	2135	2143	rVB	4244294	5978988	87.13%	7.603%
49	16.239	2146	2151	2160	rVV	1145002	1649791	24.04%	2.098%
50	17.880	2425	2430	2437	rVB	2733158	3797434	55.34%	4.829%
51	17.980	2441	2447	2455	rVV	4116920	5925278	86.35%	7.534%
52	19.080	2631	2634	2640	rVB	214978	281362	4.10%	0.358%
53	20.209	2821	2826	2836	rVB	4680002	6627859	96.59%	8.428%
54	21.968	3120	3125	3133	rVB	2966412	4156199	60.57%	5.285%
55	24.315	3516	3524	3535	rVB2	3146907	6862015	100.00%	8.725%
56	24.474	3545	3551	3561	rVB2	1918383	4079939	59.46%	5.188%

Sum of corrected areas: 78643375

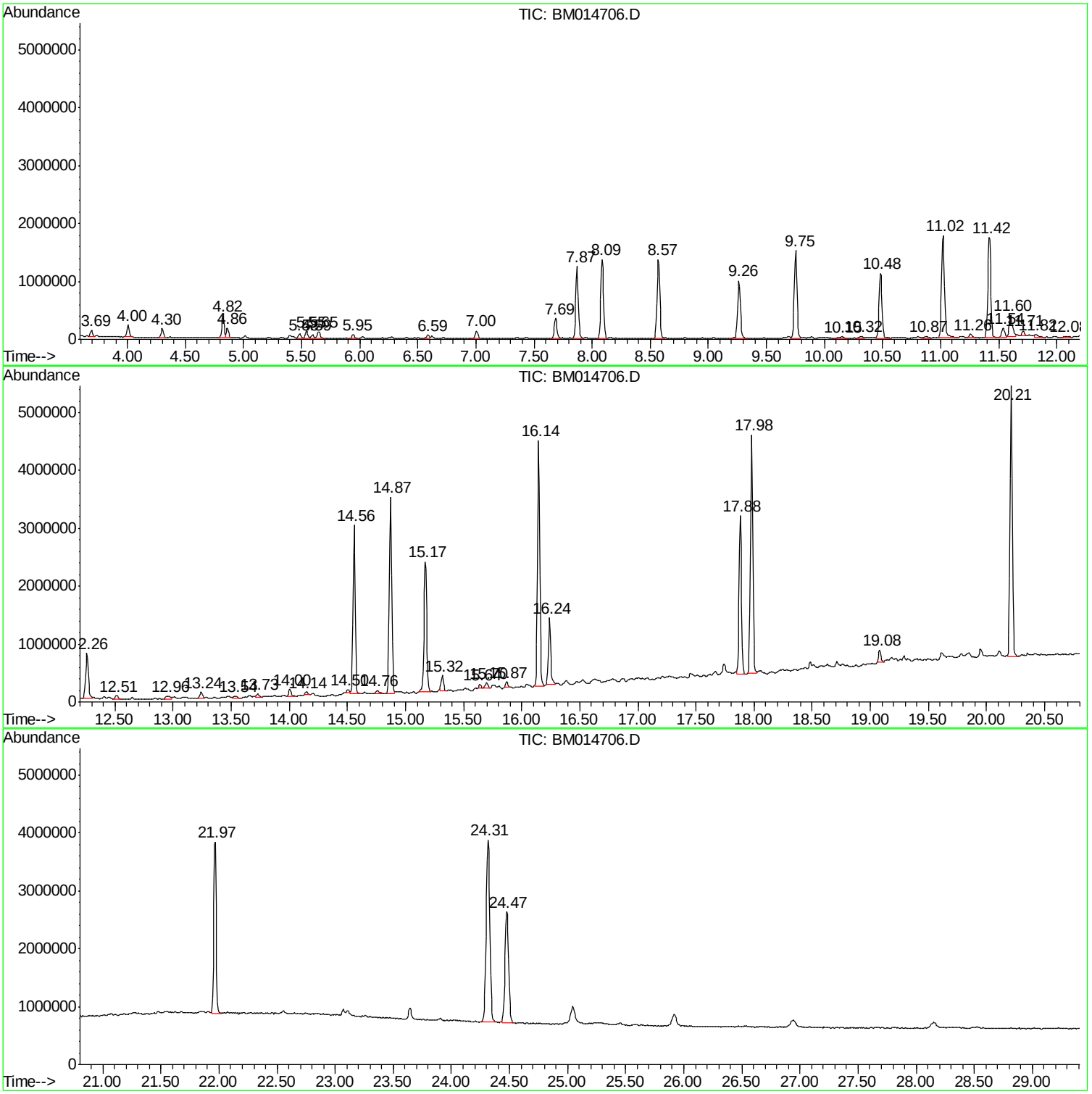
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

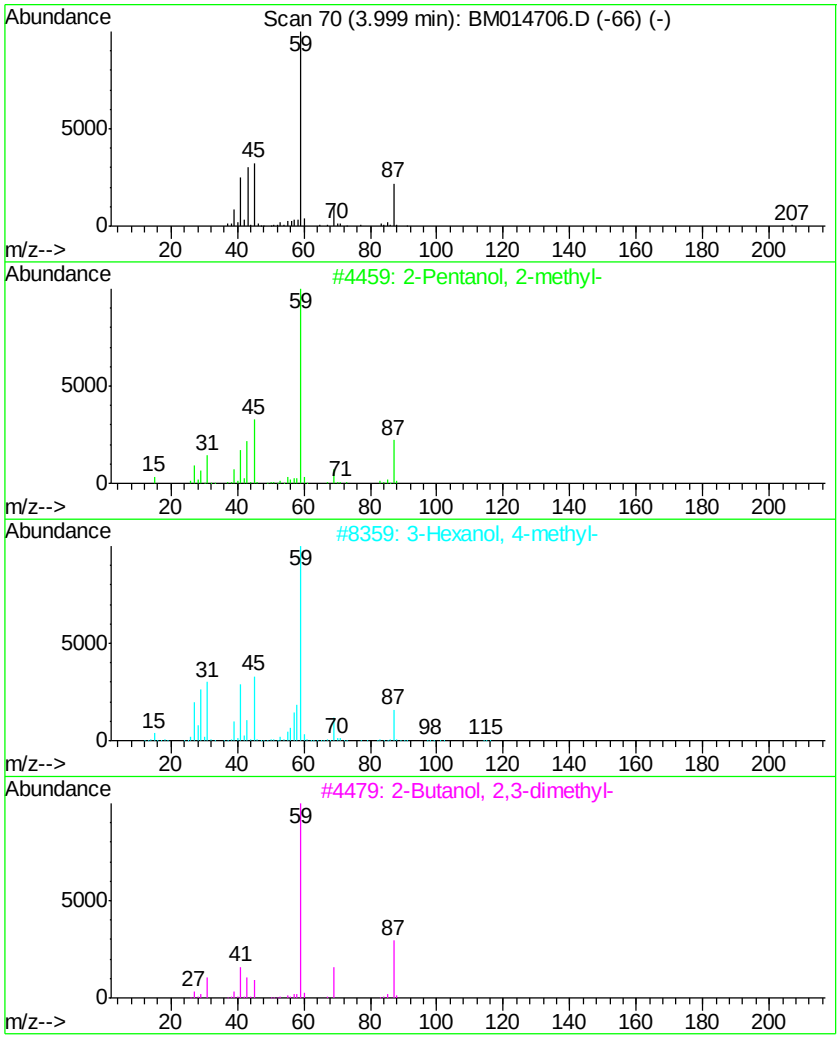
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

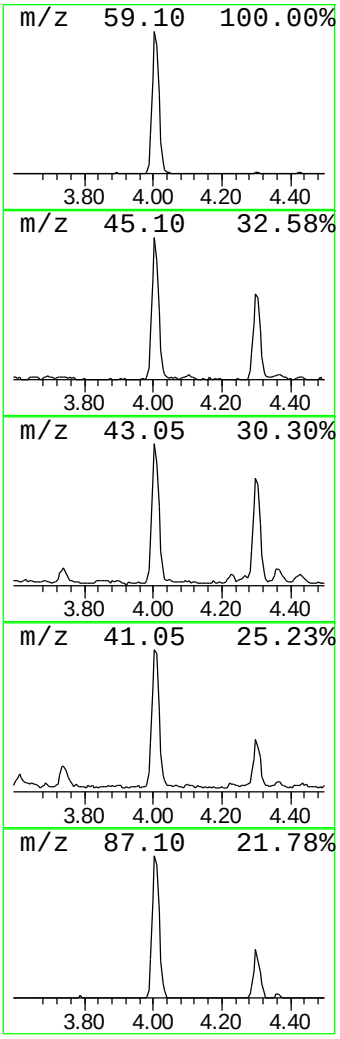
****

Peak Number 1 2-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	2.56 ng/ul	291851	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	74
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
5	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	56





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

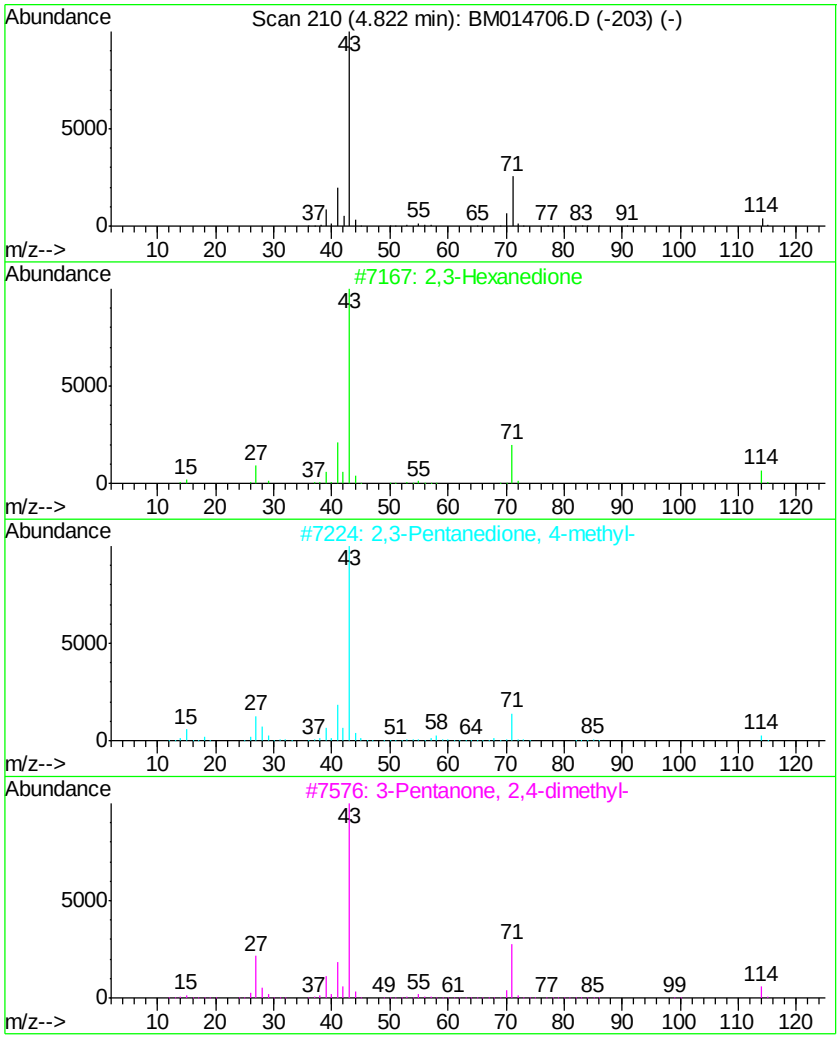
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

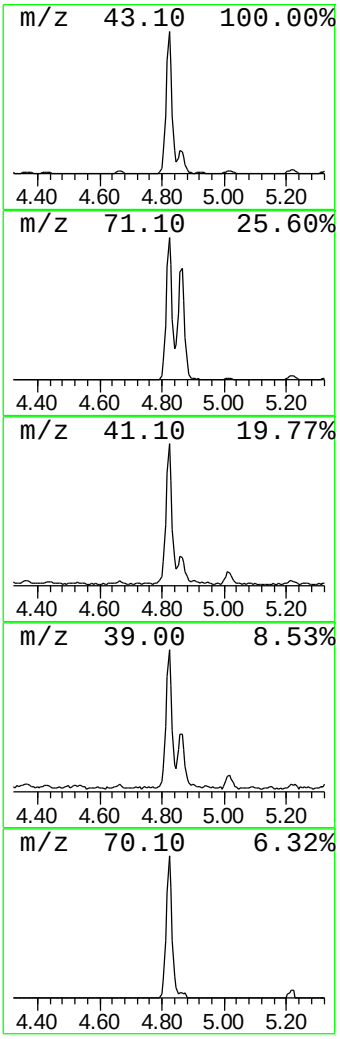
****

Peak Number 2 2,3-Hexanedione Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	4.73 ng/ul	538423	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
2	2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	64
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	43
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	42
5	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	40





Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

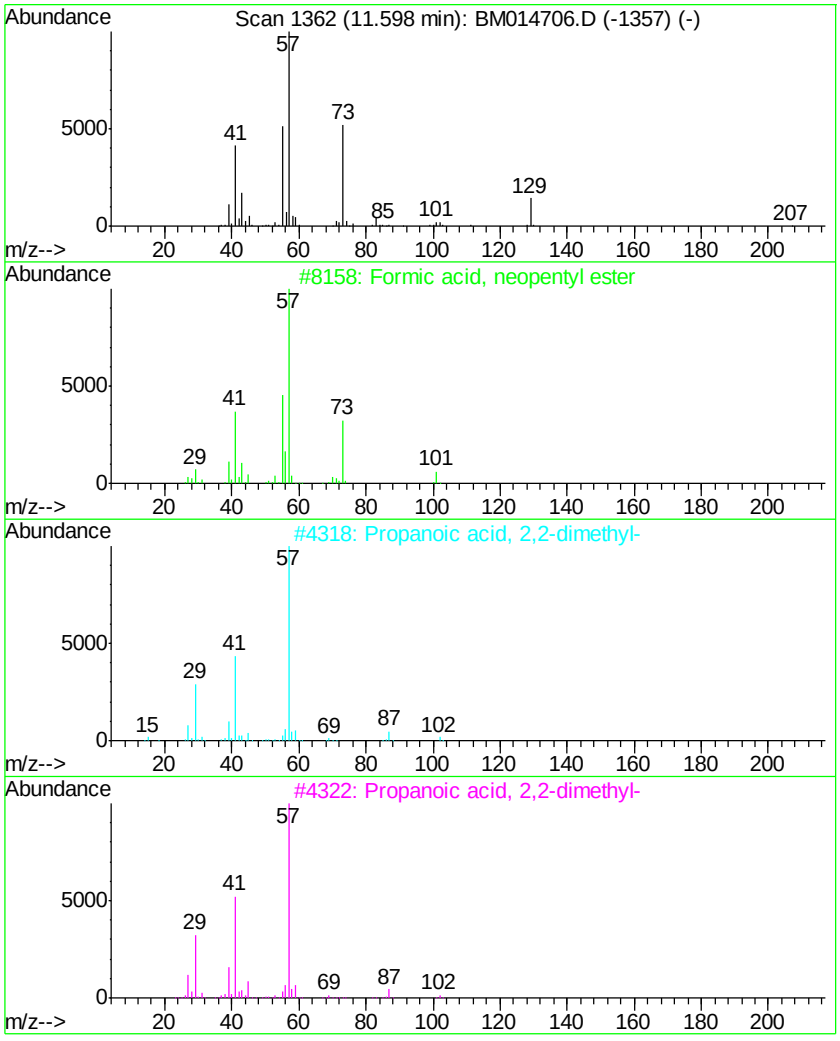
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

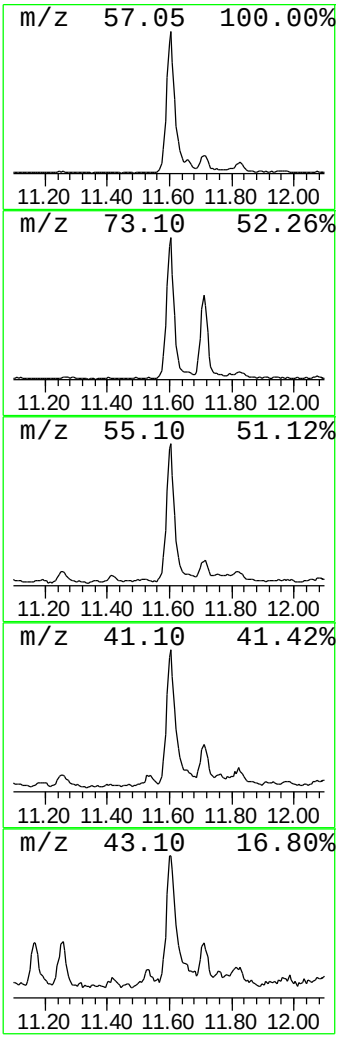
****

Peak Number 3 Formic acid, neopentyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	4.55 ng/ul	694760	Naphthalene-d8	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, neopentyl ester	116	C6H12O2	1000367-90-3	53
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	27
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	27
4	Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	23
5	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

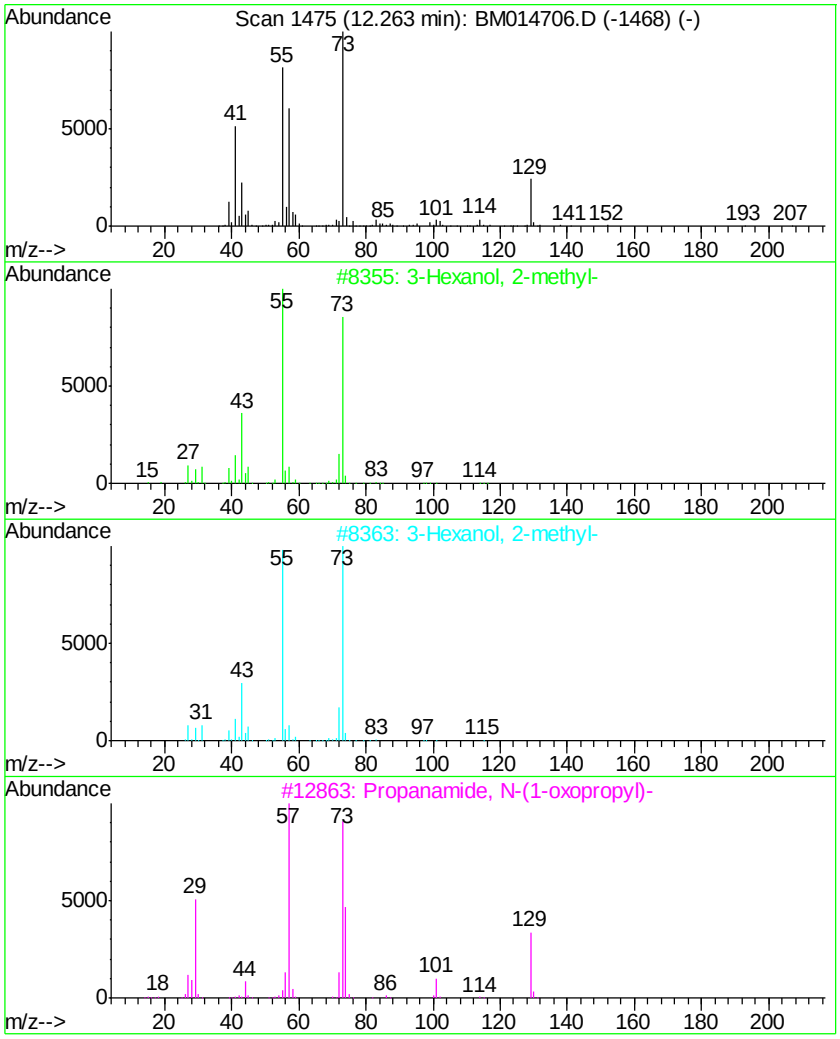
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

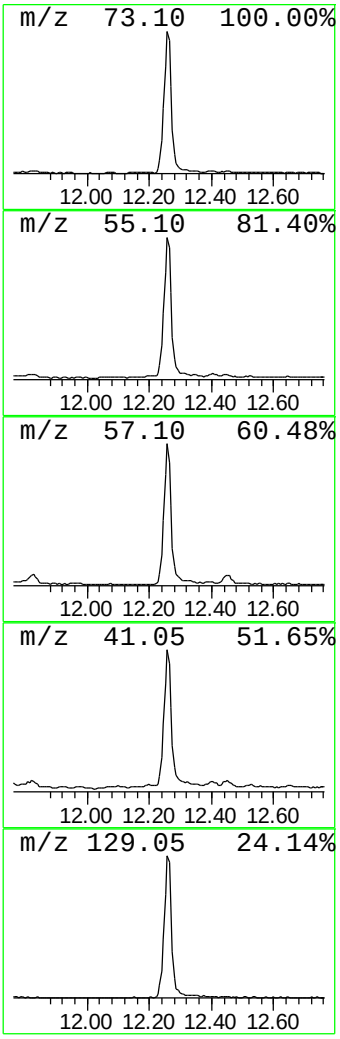
****

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	8.43 ng/ul	1286770	Naphthalene-d8	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	43
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
3	Propanamide, N-(1-oxopropyl)-	129	C6H11NO2	006050-26-6	37
4	Neopentyl isothiocyanate	129	C6H11NS	000597-97-7	35
5	2,3-Epoxyhexanol	116	C6H12O2	090528-63-5	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM041318\
Data File : BM014706.D
Acq On : 13 Apr 2018 19:06
Operator : SJ/JU
Sample : J2313-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A33

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanol, 2-met...	4.00	2.6	ng/ul	291851	1	8.57	2278170	20.0
2,3-Hexanedione	4.82	4.7	ng/ul	538423	1	8.57	2278170	20.0
Formic acid, neop...	11.60	4.5	ng/ul	694760	2	11.42	3052690	20.0
unknown-01	12.26	8.4	ng/ul	1286770	2	11.42	3052690	20.0