LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.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	3.252	42	45	54	rVB	60674	82959	1.33%	0.126%
2	3.899	153	155	163	rVB6	5274	8151	0.13%	0.012%
3	3.987	166	170	174	rVB	8586	11150	0.18%	0.017%
4	4.205	204	207	212	rVB3	4805	6360	0.10%	0.010%
5	6.775	640	644	652	rBV5	4027	6788	0.11%	0.010%
6	6.940	665	672	691	rBV	1030198	1762353	28.22%	2.682%
7	7.110	694	701	719	rBV	787555	1275994	20.43%	1.942%
8	7.310	727	735	745	rBV	1096010	1733636	27.76%	2.639%
9	7.775	807	814	822	rBV	796447	1224864	19.61%	1.864%
10	7.846	822	826	833	rVB	31111	48376	0.77%	0.074%
11	8.481	927	934	947	rBV	1251300	2044096	32.73%	3.111%
12	8.928	998	1010	1021	rBV	986882	1614905	25.86%	2.458%
13	9.369	1081	1085	1091	rVB	13572	19059	0.31%	0.029%
14	9.645	1125	1132	1146	rBV	810002	1314866	21.05%	2.001%
15	9.887	1168	1173	1183	rBV	35033	60922	0.98%	0.093%
16	10.075	1200	1205	1210	rBV3	5596	9731	0.16%	0.015%
17	10.187	1216	1224	1235	rBV	1265853	2130049	34.10%	3.242%
18	10.563	1280	1288	1295	rBV	1060765	1742576	27.90%	2.652%
19	10.698	1302	1311	1328	rBV	1220332	2096027	33.56%	3.190%
20	11.075	1370	1375	1386	rBV	13672	34443	0.55%	0.052%
21	12.151	1550	1558	1565	rBV2	17635	28167	0.45%	0.043%
22	12.686	1643	1649	1658	rBV	23799	37955	0.61%	0.058%
23	13.028	1703	1707	1710	rBV2	4567	6248	0.10%	0.010%
24	13.251	1740	1745	1750	rVB3	5064	7450	0.12%	0.011%
25	13.633	1805	1810	1817	rBV	64780	87054	1.39%	0.132%
26	13.822	1834	1842	1846	rBV	2086345	2818857	45.13%	4.290%
27	13.869	1846	1850	1855	rVB	378925	509897	8.16%	0.776%
28	14.104	1880	1890	1900	rBV	2612041	3692852	59.13%	5.621%
29	14.316	1922	1926	1932	rVB3	6626	10950	0.18%	0.017%
30	14.410	1936	1942	1949	rVV	1521939	2231815	35.73%	3.397%
31	14.604	1968	1975	1994	rBV	957886	1393593	22.31%	2.121%
32	14.839	2009	2015	2029	rBV	198644	300808	4.82%	0.458%
33	15.216	2076	2079	2085	rBV2	7254	11910	0.19%	0.018%
34	15.274	2085	2089	2094	rVB3	10474	14435	0.23%	0.022%

LSC Area Percent Report

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Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Title : SVOA CALIBRATION

35	15.404	2104	2111	2122	rBV	3203356	4400786	70.46%	6.698%
36	15.522	2124	2131	2143	rBV	849644	1188014	19.02%	1.808%
37	15.645	2147	2152	2156	rBV	31945	43705	0.70%	0.067%
38	16.133	2230	2235	2238	rBV2	9475	12883	0.21%	0.020%
39	16.186	2241	2244	2248	rVB3	9489	12962	0.21%	0.020%
40	16.557	2301	2307	2314	rBV	54547	78968	1.26%	0.120%
41	16.921	2365	2369	2383	rVB3	10059	22413	0.36%	0.034%
42	17.151	2402	2408	2418	rVV2	1821560	2495251	39.95%	3.798%
43	17.251	2418	2425	2435	rVV	3285846	4540860	72.70%	6.911%
44	17.321	2435	2437	2444	rVB6	7532	13088	0.21%	0.020%
45	17.439	2454	2457	2462	rBV	5670	6336	0.10%	0.010%
46	17.539	2468	2474	2484	rBV6	19232	36199	0.58%	0.055%
47	17.657	2491	2494	2500	rBV	7731	9512	0.15%	0.014%
48	17.915	2535	2538	2545	rBV5	7652	13003	0.21%	0.020%
49	17.986	2547	2550	2553	rVB3	7359	9367	0.15%	0.014%
50	18.051	2555	2561	2571	rBV	366540	526496	8.43%	0.801%
51	18.345	2609	2611	2615	rBV3	7612	11674	0.19%	0.018%
52	18.480	2631	2634	2637	rVB5	19767	21477	0.34%	0.033%
53	18.757	2677	2681	2685	rBV3	15242	17151	0.27%	0.026%
54	18.804	2685	2689	2692	rBV	22192	26734	0.43%	0.041%
55	18.945	2711	2713	2716	rVV4	7366	7863	0.13%	0.012%
56	18.980	2717	2719	2725	rVB3	13024	17213	0.28%	0.026%
57	19.180	2748	2753	2756	rBV	47825	68344	1.09%	0.104%
58	19.204	2756	2757	2761	rVB2	14625	17369	0.28%	0.026%
59	19.327	2774	2778	2788	rBV	129887	202974	3.25%	0.309%
60	19.427	2792	2795	2800	rVB	31145	45156	0.72%	0.069%
61	19.545	2809	2815	2821	rBV	4127330	5545197	88.78%	8.440%
62	19.604	2821	2825	2831	rVB2	60851	93378	1.50%	0.142%
63	19.886	2868	2873	2876	rBV	637197	672200	10.76%	1.023%
64	19.921	2876	2879	2884	rVB	1010843	1080354	17.30%	1.644%
65	20.068	2900	2904	2906	rBV4	16746	25177	0.40%	0.038%
66	20.098	2906	2909	2913	rVB	36338	38203	0.61%	0.058%
67	20.592	2990	2993	2996	rBV	50840	54375	0.87%	0.083%
68	20.862	3035	3039	3041	rBV	309078	333745	5.34%	0.508%
69	20.892	3041	3044	3050	rVB	513510	537664	8.61%	0.818%
70	21.051	3067	3071	3081	rBV	622249	874488	14.00%	1.331%
71	21.333	3114	3119	3125	rBV	2420269	2937343	47.03%	4.471%

LSC Area Percent Report

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Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Title : SVOA CALIBRATION

72	21.492	3143	3146	3150	rBV	129607	133359	2.14%	0.203%
73	21.733	3183	3187	3189	rBV	195528	227464	3.64%	0.346%
74	21.762	3189	3192	3198	rVB	281158	309924	4.96%	0.472%
75	21.927	3217	3220	3231	rBV2	153738	260500	4.17%	0.396%
76	22.392	3296	3299	3304	rBV	162001	203642	3.26%	0.310%
77	22.662	3342	3345	3348	rBV	132460	174671	2.80%	0.266%
78	22.703	3349	3352	3359	rVB	233770	309704	4.96%	0.471%
79	22.909	3383	3387	3392	rVB	178048	250369	4.01%	0.381%
80	23.445	3471	3478	3490	rVB	3330388	6245763	100.00%	9.506%
81	23.586	3495	3502	3513	rVB	1726987	3168691	50.73%	4.823%

Sum of corrected areas: 65701305

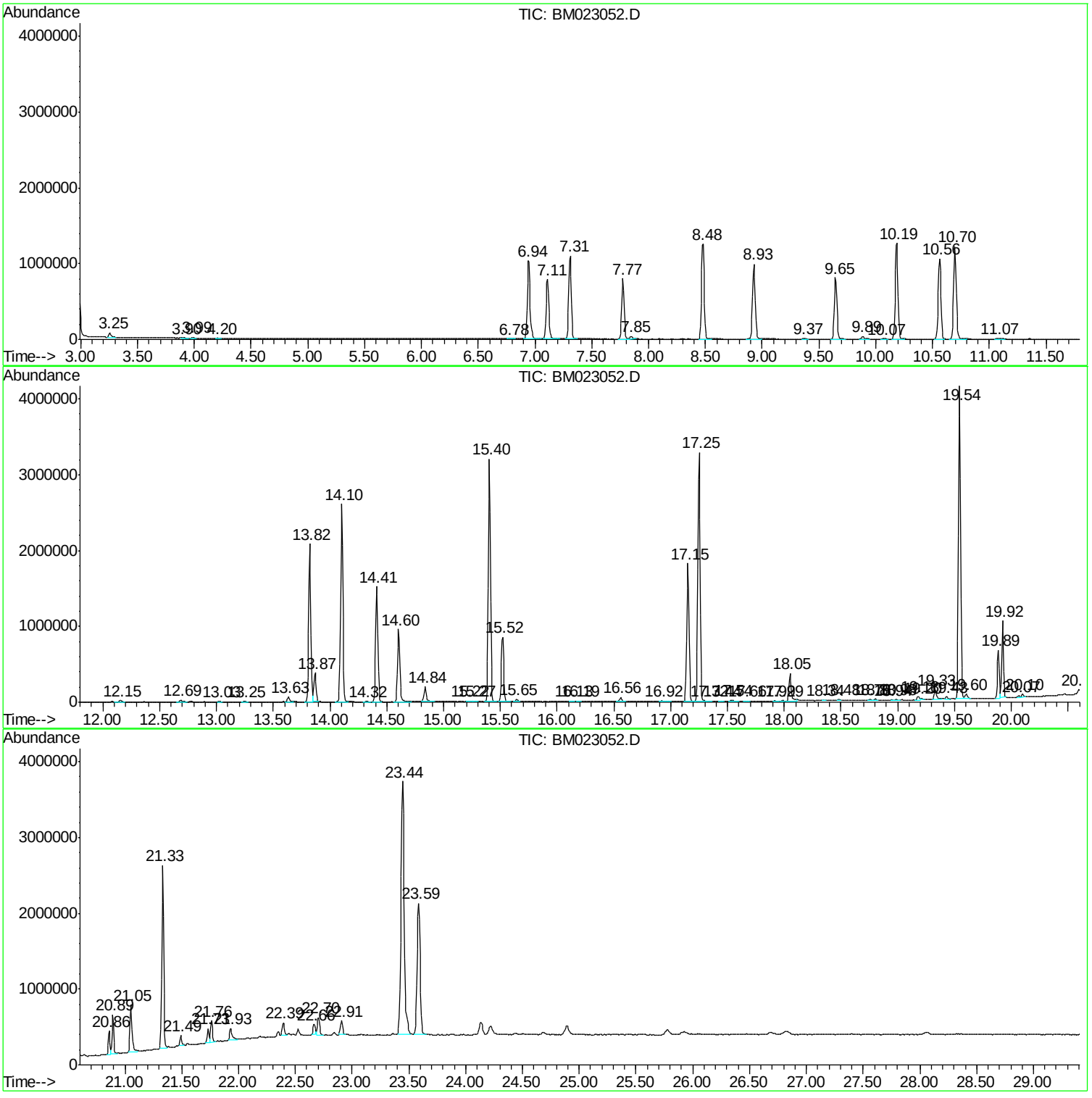
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

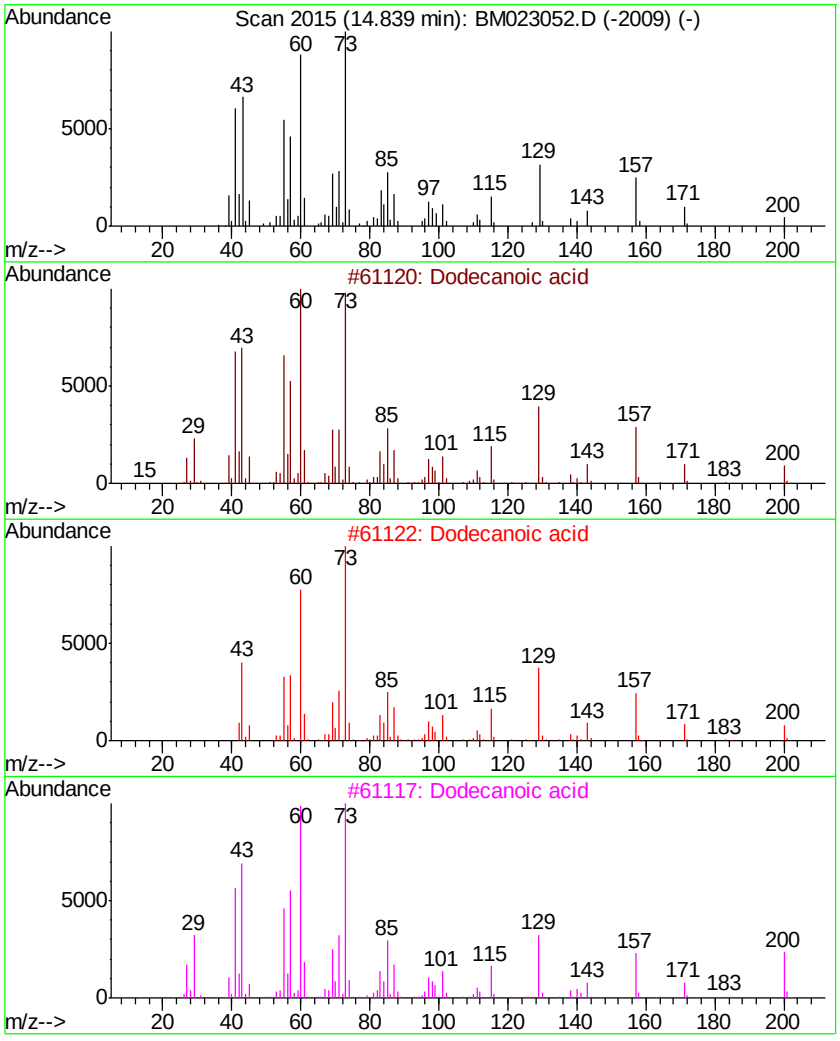
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

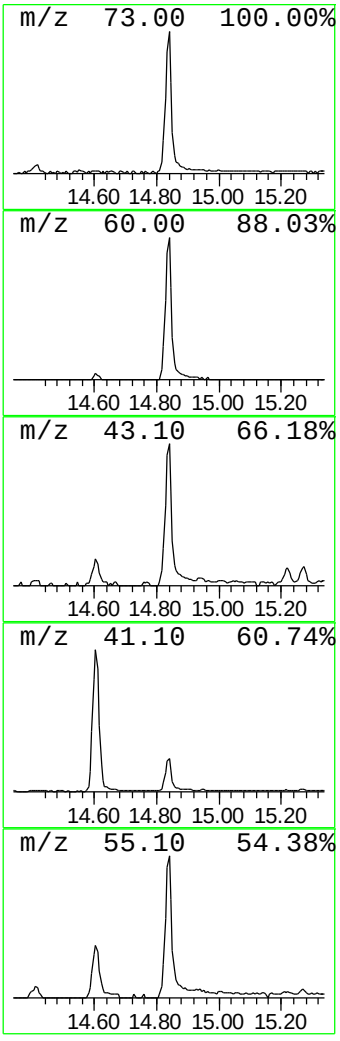
****

Peak Number 1 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.70 ng/ul	300808	Acenaphthene-d10	14.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	97
2	Dodecanoic acid	200	C12H24O2	000143-07-7	91
3	Dodecanoic acid	200	C12H24O2	000143-07-7	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

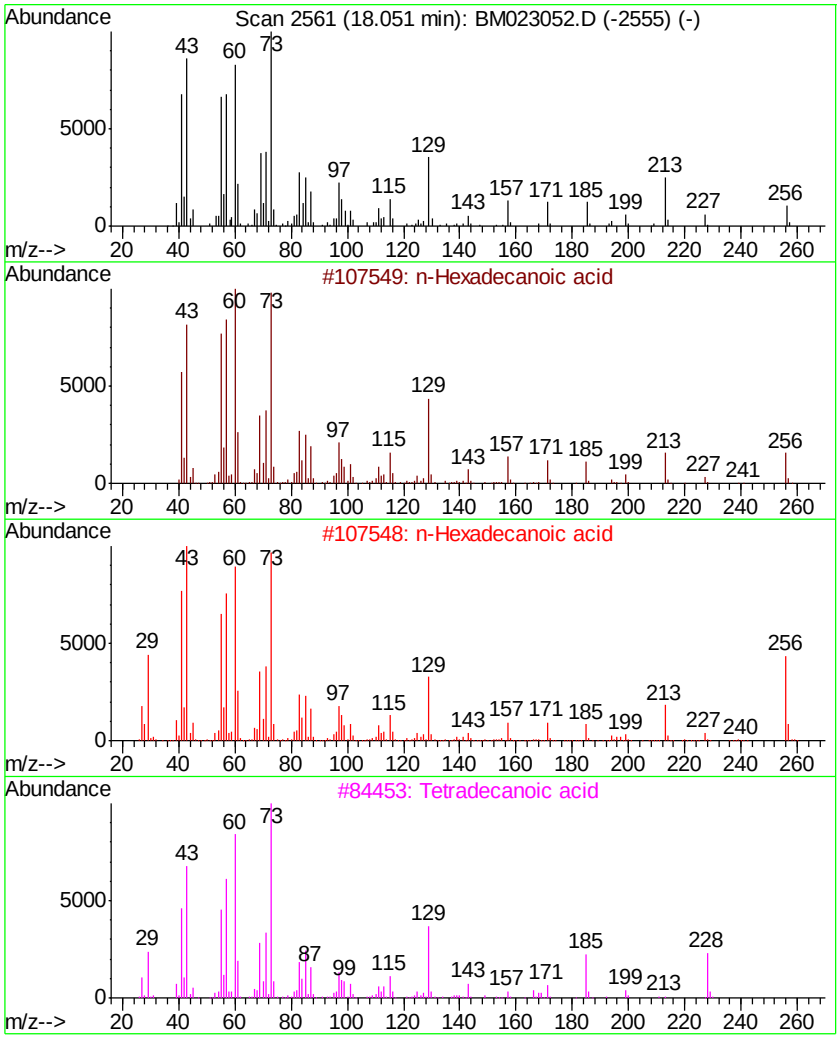
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

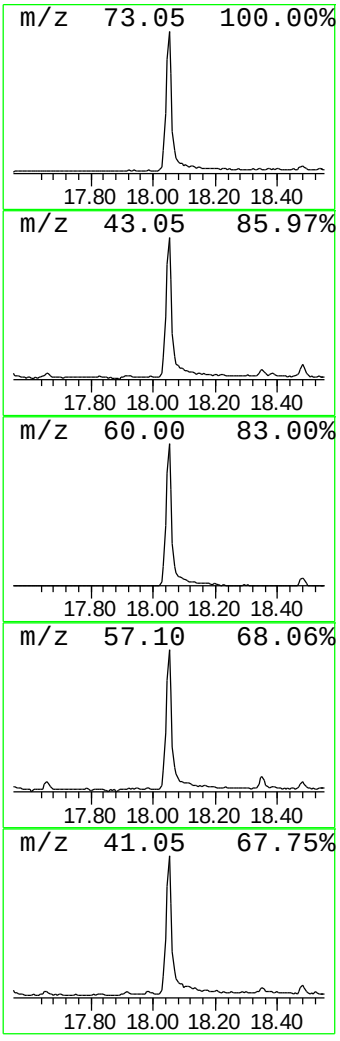
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	4.22 ng/ul	526496	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

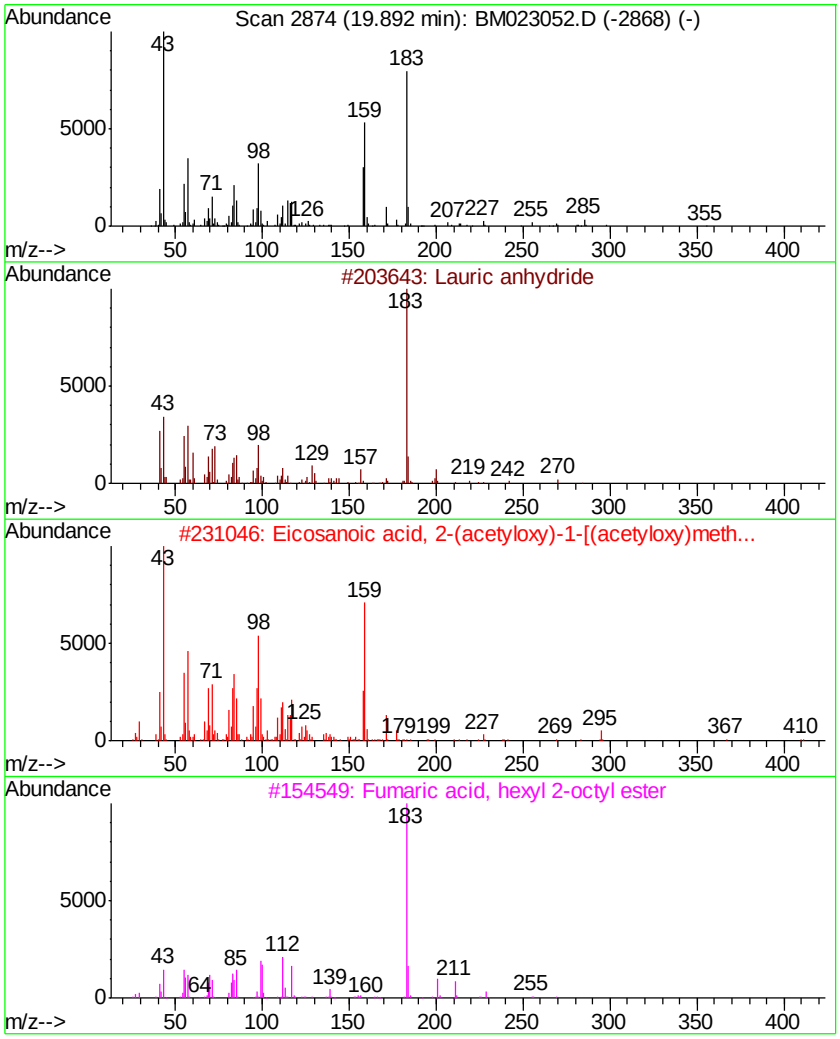
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

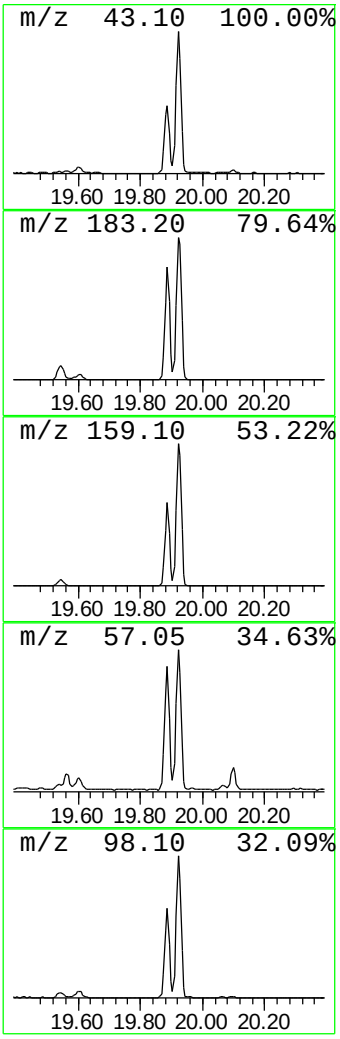
****

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	4.58 ng/ul	672200	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauric anhydride	382	C24H46O3	000645-66-9	35
2	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	27
3	Fumaric acid, hexyl 2-octyl ester	312	C18H32O4	1000339-16-6	25
4	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	25
5	Dodecanoic acid, pentafluorophen...	366	C18H23F5O2	1000360-54-1	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

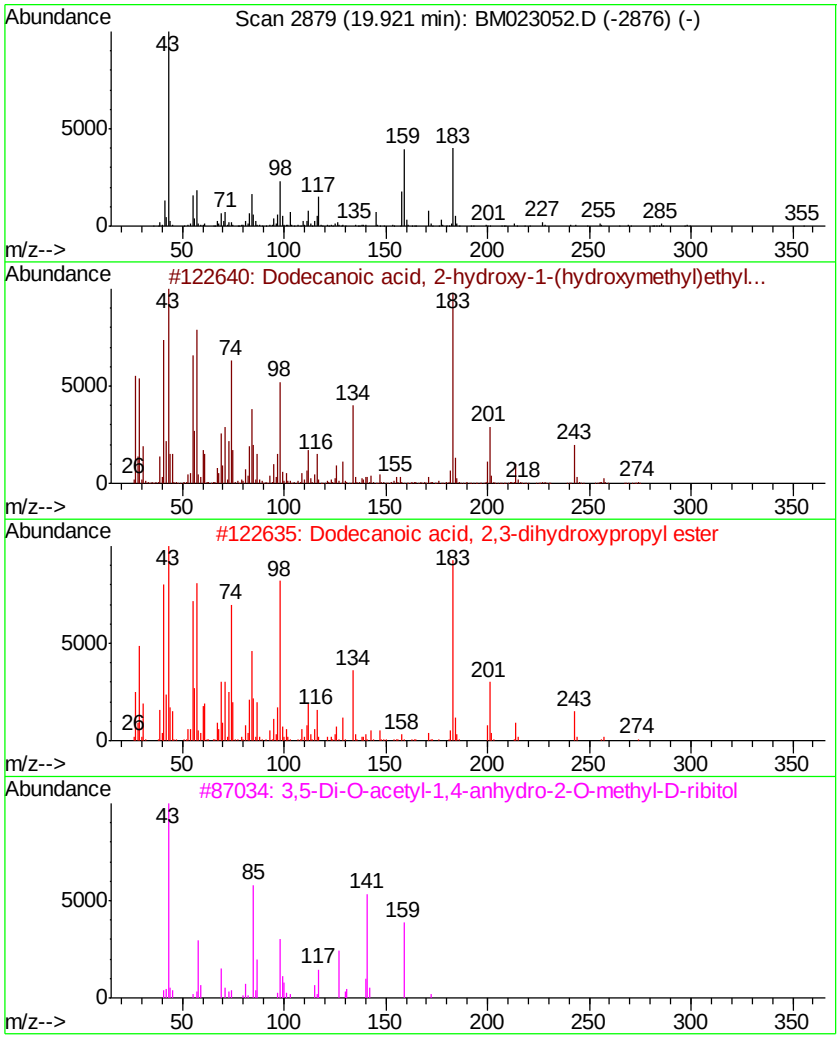
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

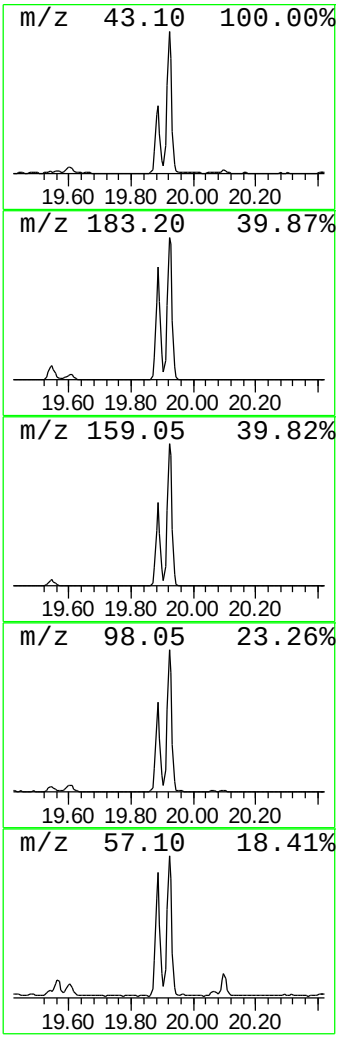
****

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	7.36 ng/ul	1080350	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	35
2	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	22
3	3,5-Di-O-acetyl-1,4-anhydro-2-O-...	232	C10H16O6	1000357-23-2	17
4	Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12
5	Acetic acid, 6-iodo-9-oxabicyclo...	310	C10H15IO3	1000190-80-0	9





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Acq On : 08 Oct 2019 19:11
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Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

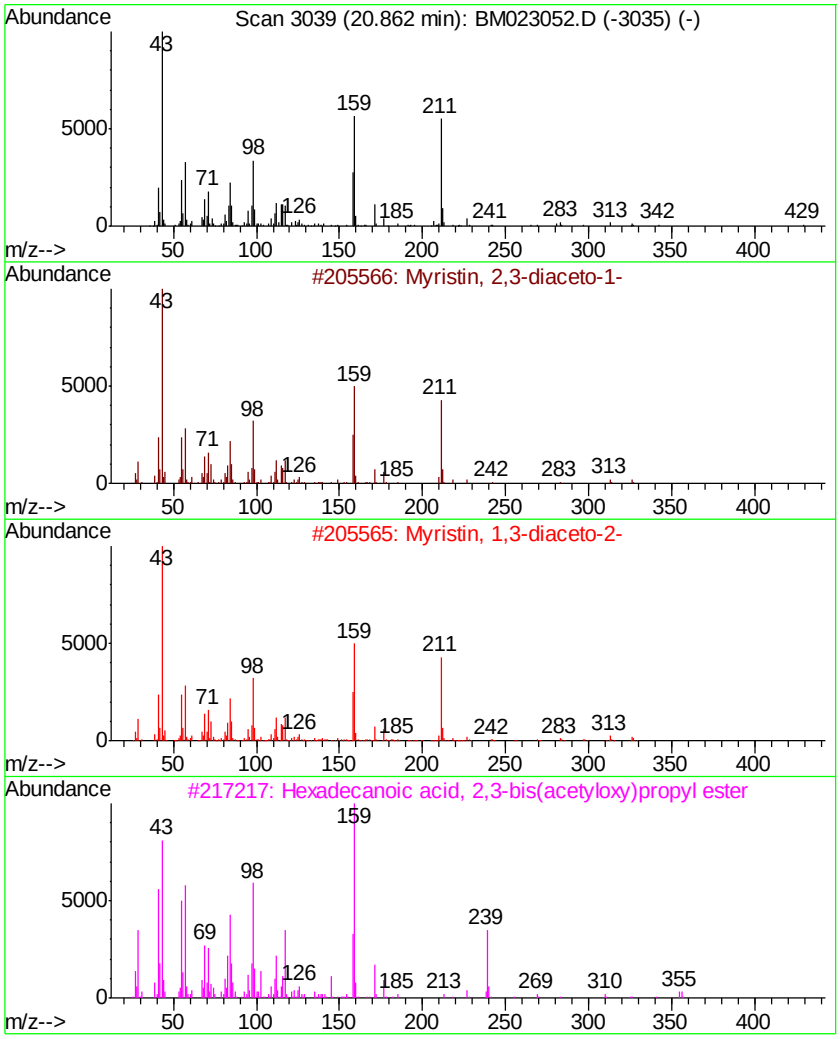
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

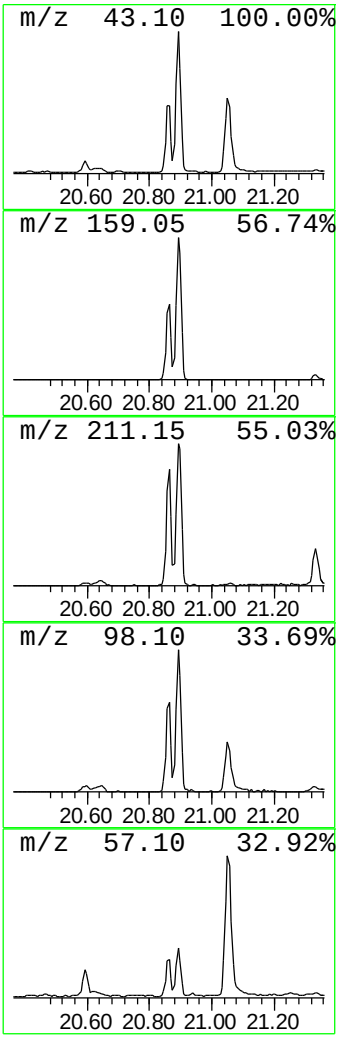
****

Peak Number 5 Myristin, 2,3-diaceto-1- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.27 ng/ul	333745	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	91
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
3	Hexadecanoic acid, 2,3-bis(acetv...	414	C23H42O6	055268-70-7	49
4	6,7-Dihydro-2-dimethylamino-8-me...	211	C8H13N5O2	079845-30-0	22
5	2,5-Difluorobenzoic acid, decyl ...	298	C17H24F2O2	1000338-80-9	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

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

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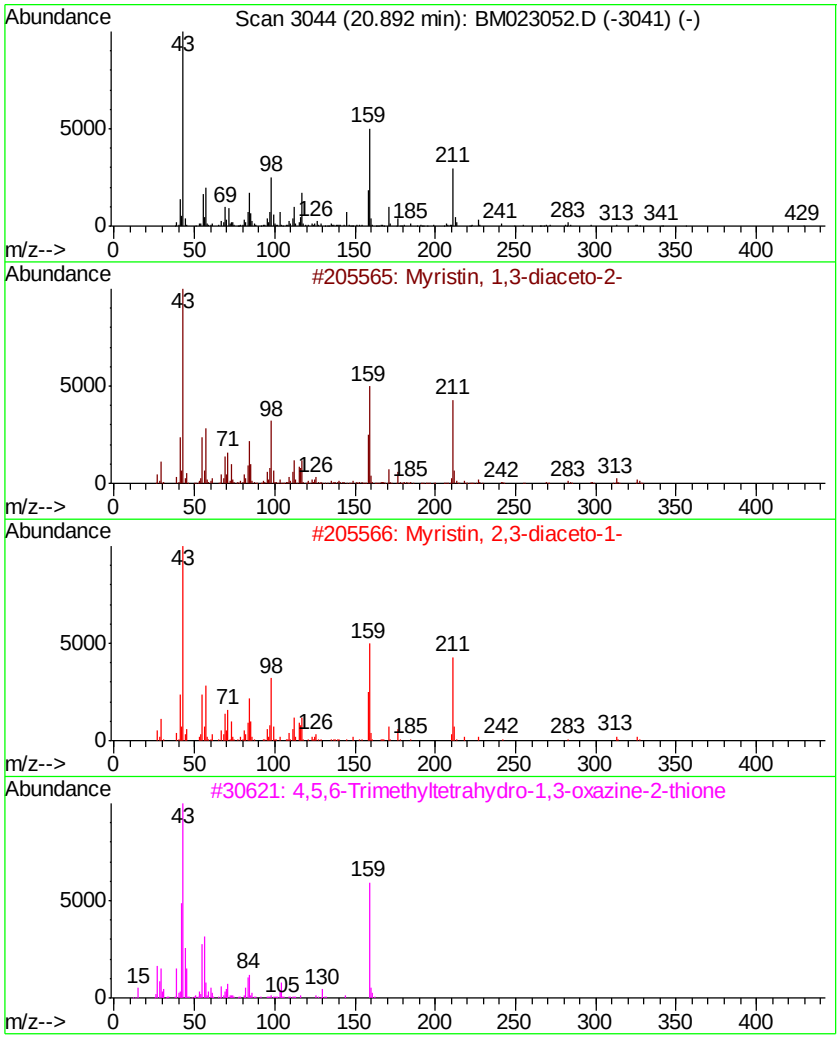
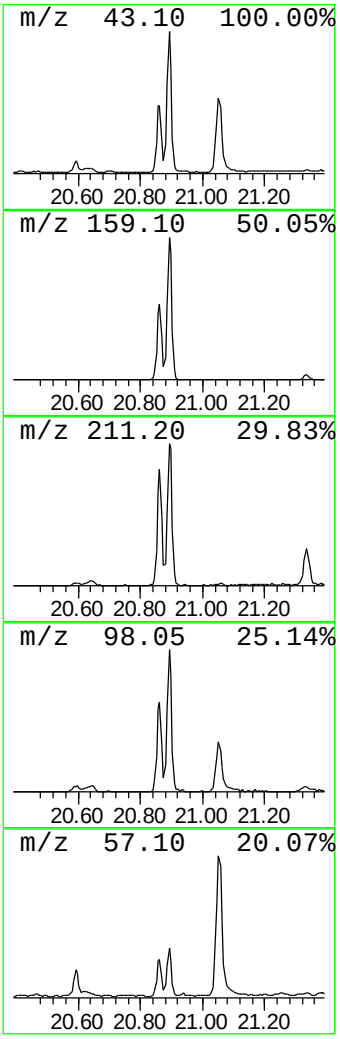
Peak Number 6 Myristin, 1,3-diaceto-2- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.89	3.66 ng/ul	537664	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	68
2	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	64
3	4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	22
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	12
5	Thioacetic acid, S-(5-acetylthio...	234	C9H14O3S2	1000185-15-4	10





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Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

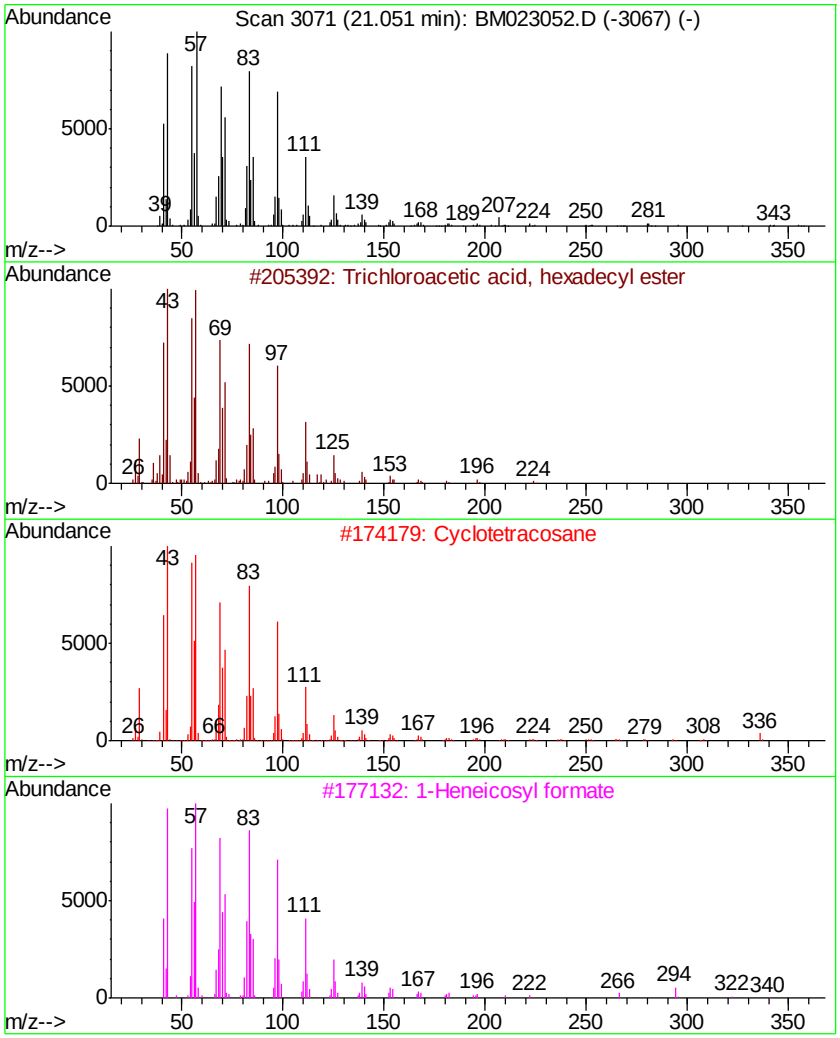
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

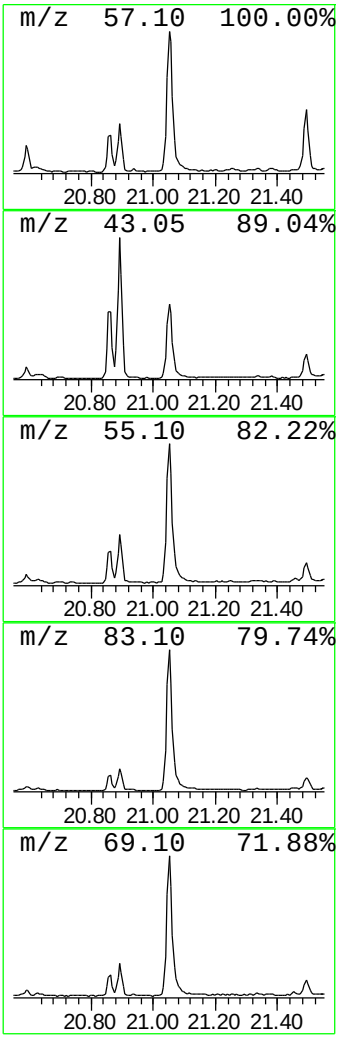
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	5.95 ng/ul	874488	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

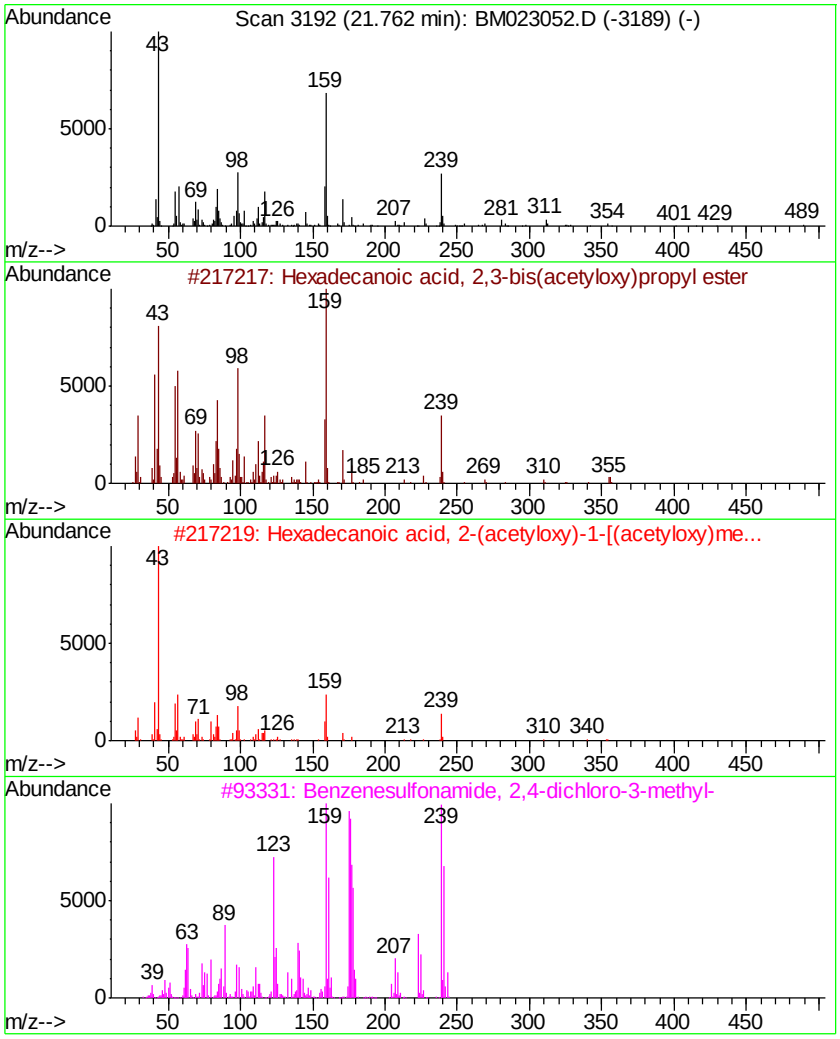
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

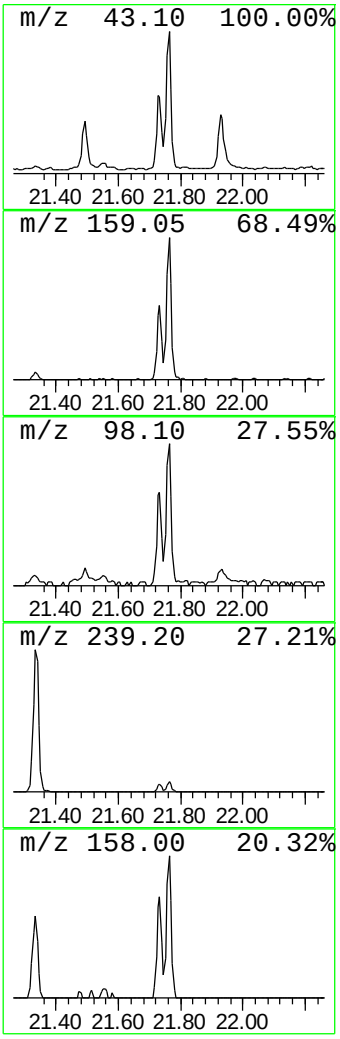
****

Peak Number 8 Hexadecanoic acid, 2,3-bis(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.76	2.11 ng/ul	309924	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2,3-bis(acetyl...	414	C23H42O6	055268-70-7	52
2	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	38
3	Benzenesulfonamide, 2,4-dichloro...	239	C7H7Cl2NO2S	1000277-29-3	27
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	22
5	2,5-Difluorobenzoic acid, decyl ...	298	C17H24F2O2	1000338-80-9	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM100819\
Data File : BM023052.D
Acq On : 08 Oct 2019 19:11
Operator : JU
Sample : K5056-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.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
Dodecanoic acid	14.84	2.7	ng/ul	300808	3	14.41	2231820	20.0
n-Hexadecanoic acid	18.05	4.2	ng/ul	526496	4	17.15	2495250	20.0
unknown-01	19.89	4.6	ng/ul	672200	5	21.33	2937340	20.0
unknown-02	19.92	7.4	ng/ul	1080350	5	21.33	2937340	20.0
Myristin, 2,3-dia...	20.86	2.3	ng/ul	333745	5	21.33	2937340	20.0
Myristin, 1,3-dia...	20.89	3.7	ng/ul	537664	5	21.33	2937340	20.0
Trichloroacetic a...	21.05	6.0	ng/ul	874488	5	21.33	2937340	20.0
Hexadecanoic acid...	21.76	2.1	ng/ul	309924	5	21.33	2937340	20.0