LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010628.D
Acq On : 21 Jun 2017 18:16
Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5E22

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-BM062017.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	6.646	633	639	648	rVB	210140	325777	18.63%	1.652%
2	6.816	662	668	676	rBB	158396	227783	13.03%	1.155%
3	7.005	694	700	706	rBB	222314	336133	19.22%	1.704%
4	7.463	772	778	785	rBV	233189	345228	19.74%	1.750%
5	8.169	892	898	905	rBB	277053	428036	24.48%	2.170%
6	8.604	965	972	979	rBB	216852	338564	19.36%	1.716%
7	9.322	1088	1094	1100	rBV	207214	313338	17.92%	1.589%
8	9.851	1178	1184	1193	rBB	325263	496519	28.40%	2.517%
9	10.228	1241	1248	1252	rBV	332890	525277	30.04%	2.663%
10	10.275	1252	1256	1264	rVV	178116	282039	16.13%	1.430%
11	10.369	1266	1272	1281	rBB	133919	218823	12.51%	1.109%
12	11.898	1526	1532	1537	rBV2	17675	26348	1.51%	0.134%
13	13.539	1804	1811	1815	rBV	635548	879941	50.32%	4.461%
14	13.581	1815	1818	1826	rVB	197044	265868	15.20%	1.348%
15	13.804	1849	1856	1867	rVB	647088	920959	52.67%	4.669%
16	14.116	1903	1909	1916	rBV3	541026	801578	45.84%	4.064%
17	14.181	1916	1920	1924	rVB2	19147	26410	1.51%	0.134%
18	14.322	1937	1944	1952	rBV	309196	421238	24.09%	2.136%
19	14.516	1972	1977	1981	rBV2	23518	31062	1.78%	0.157%
20	14.610	1989	1993	1999	rBV	21724	30131	1.72%	0.153%
21	14.880	2034	2039	2043	rBV	29704	39503	2.26%	0.200%
22	15.116	2073	2079	2085	rBV	848794	1176105	67.26%	5.962%
23	15.169	2085	2088	2095	rVB2	25126	34127	1.95%	0.173%
24	15.239	2095	2100	2109	rBB	308879	391740	22.40%	1.986%
25	15.869	2202	2207	2210	rBV2	17667	21496	1.23%	0.109%
26	16.869	2371	2377	2382	rBV2	795213	1077324	61.61%	5.462%
27	16.910	2382	2384	2388	rVV	68825	80874	4.63%	0.410%
28	16.969	2388	2394	2407	rVB	1036572	1393324	79.68%	7.064%
29	17.274	2442	2446	2453	rVB	44534	60442	3.46%	0.306%
30	17.792	2528	2534	2541	rBV	168457	218530	12.50%	1.108%
31	18.563	2661	2665	2669	rBV4	14692	17831	1.02%	0.090%
32	18.939	2725	2729	2739	rVB2	45435	77309	4.42%	0.392%
33	19.092	2750	2755	2761	rBV	110596	134737	7.71%	0.683%
34	19.280	2781	2787	2795	rBV	1289026	1728050	98.82%	8.761%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5E22

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-BM062017.M
Title : SVOA CALIBRATION

35	19.368	2796	2802	2808	rVB7	17399	31196	1.78%	0.158%
36	19.657	2847	2851	2854	rBV2	162085	168649	9.64%	0.855%
37	19.698	2854	2858	2863	rVB	271265	321069	18.36%	1.628%
38	20.639	3014	3018	3021	rBV4	71358	89635	5.13%	0.454%
39	20.674	3021	3024	3028	rVB	143580	154310	8.82%	0.782%
40	20.821	3045	3049	3057	rVB	133419	154049	8.81%	0.781%
41	21.086	3088	3094	3098	rBV	1125989	1430236	81.79%	7.251%
42	21.504	3161	3165	3168	rBV3	50648	67362	3.85%	0.342%
43	21.533	3168	3170	3174	rVB3	79137	85660	4.90%	0.434%
44	22.251	3290	3292	3297	rVB4	27456	31614	1.81%	0.160%
45	22.392	3313	3316	3319	rBV4	44042	55036	3.15%	0.279%
46	22.433	3319	3323	3327	rVB4	77025	105057	6.01%	0.533%
47	22.615	3351	3354	3359	rVB5	30816	40286	2.30%	0.204%
48	23.092	3429	3435	3442	rVV2	1051186	1748613	100.00%	8.865%
49	23.151	3442	3445	3450	rVB4	46281	57881	3.31%	0.293%
50	23.227	3451	3458	3465	rVB	714495	1299479	74.31%	6.588%
51	23.762	3545	3549	3553	rVB3	51119	69196	3.96%	0.351%
52	24.462	3664	3668	3676	rVB8	57964	123454	7.06%	0.626%

Sum of corrected areas: 19725226

LSC Report - Integrated Chromatogram

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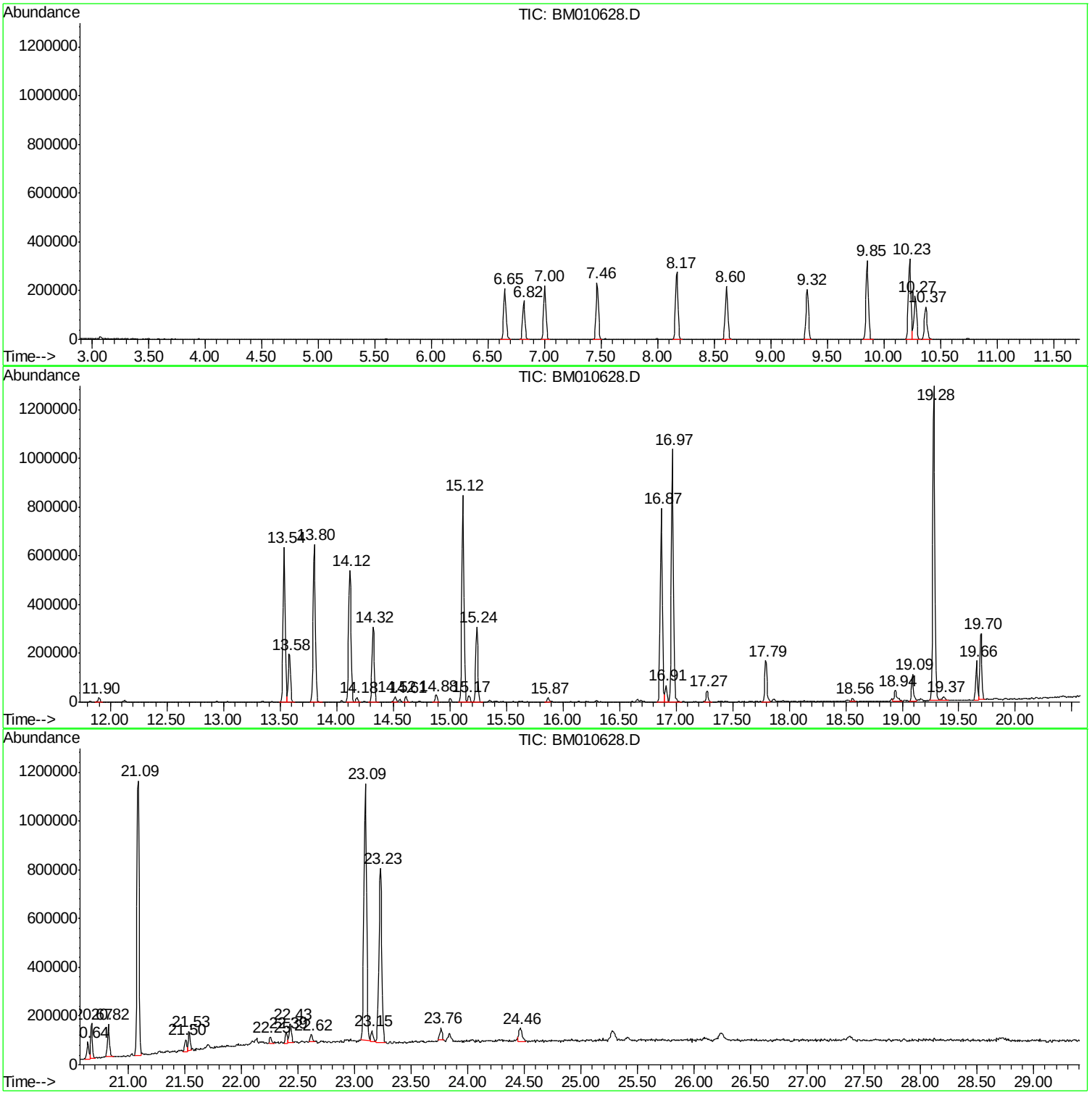
Data File : BM010628.D
Acq On : 21 Jun 2017 18:16
Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F5E22

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010628.D
Acq On : 21 Jun 2017 18:16
Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5E22

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

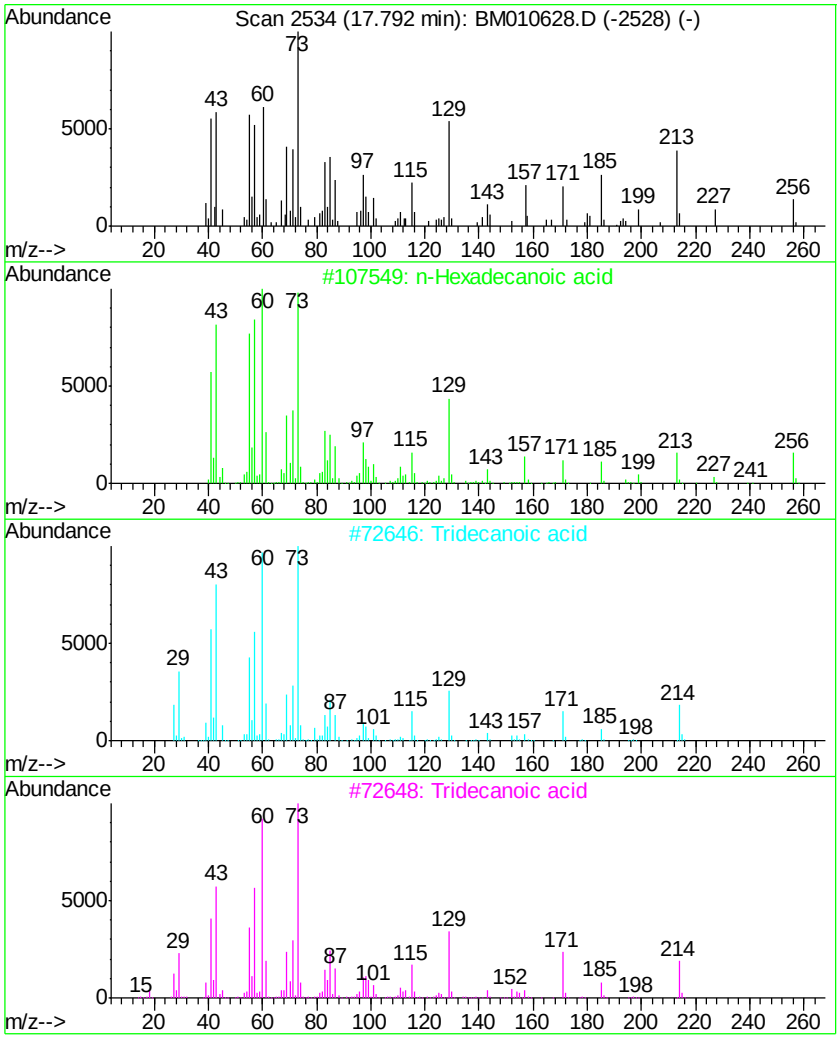
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

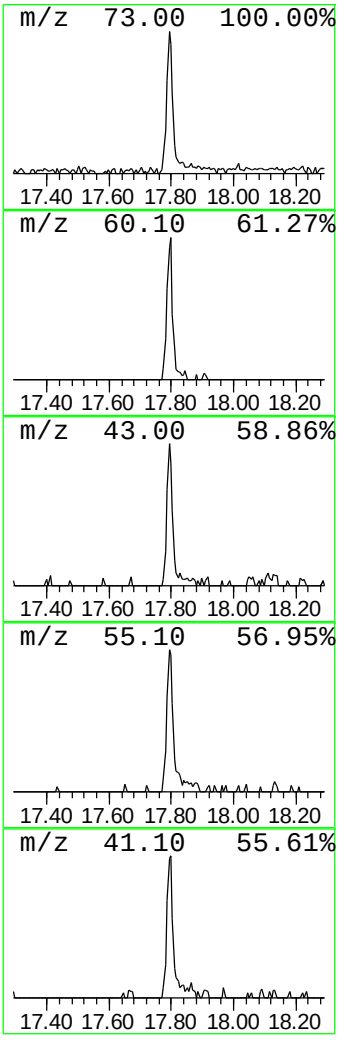
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	4.06 ng/ul	218530	Phenanthrene-d10	16.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	49





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010628.D
Acq On : 21 Jun 2017 18:16
Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5E22

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

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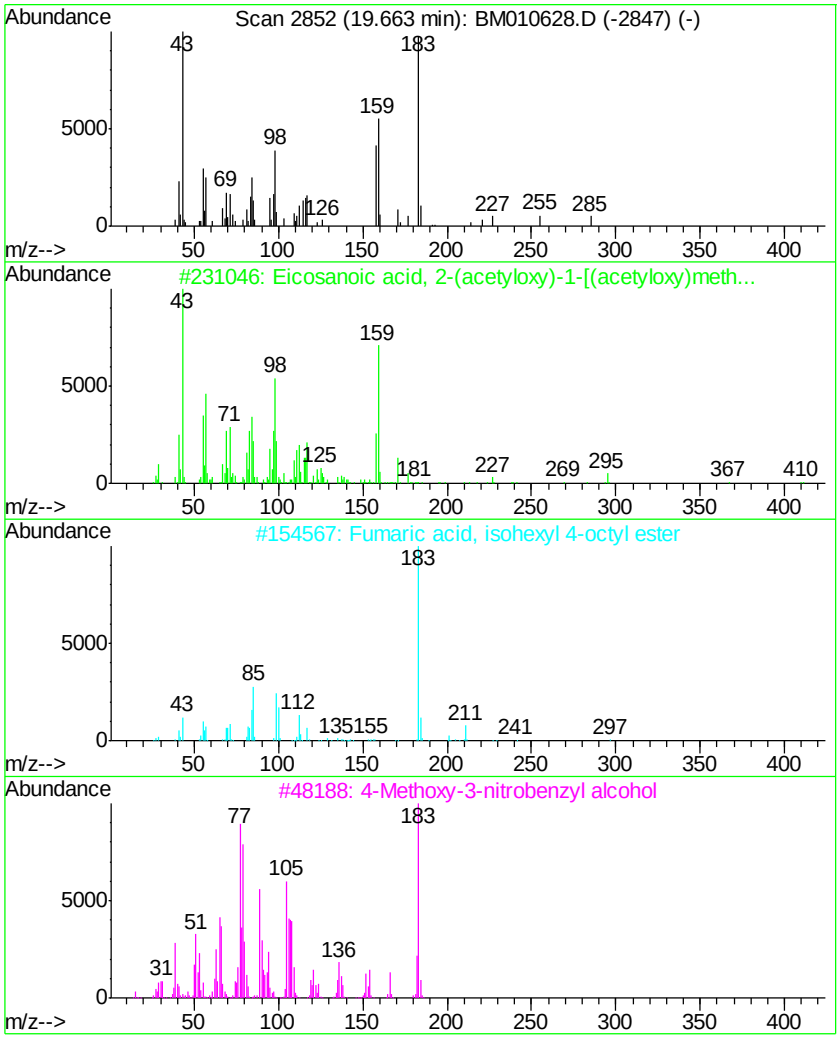
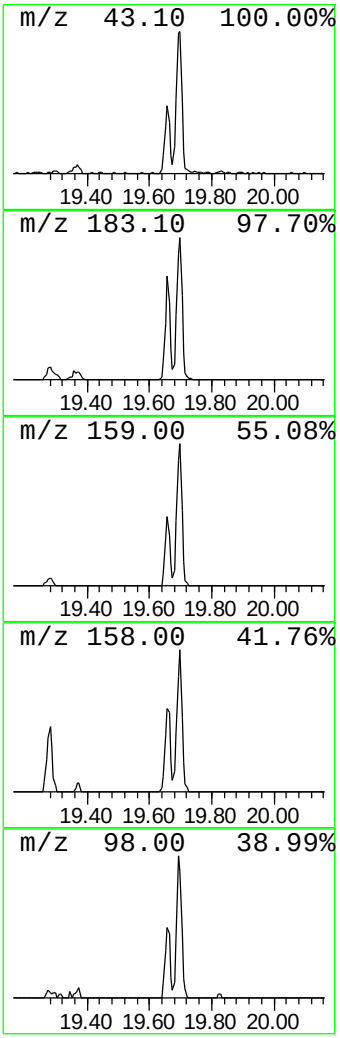
Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.66	2.36 ng/ul	168649	Chrysene-d12	21.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	43
2	Fumaric acid, isohexyl 4-octyl e...	312	C18H32O4	1000339-21-6	35
3	4-Methoxy-3-nitrobenzyl alcohol	183	C8H9NO4	041870-24-0	27
4	Dodecanoic acid, 2,4,5-trichloro...	378	C18H25Cl3O2	1000360-54-9	27
5	Cyclohexane-1,3-dione, 5,5-dimet...	377	C21H35N3O3	1000270-84-8	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062117\
Data File : BM010628.D
Acq On : 21 Jun 2017 18:16
Operator : SJ/JU
Sample : I3653-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5E22

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

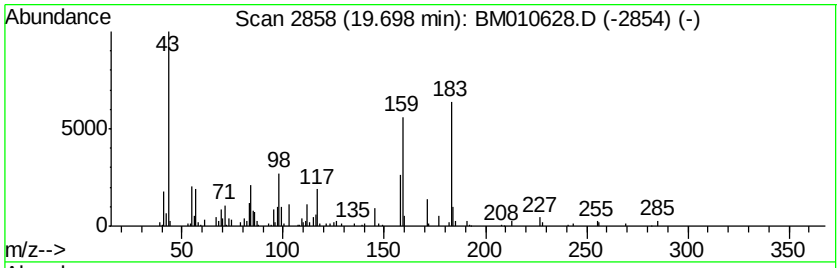
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

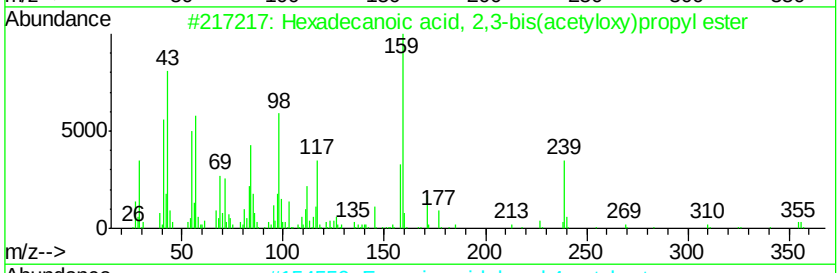
****

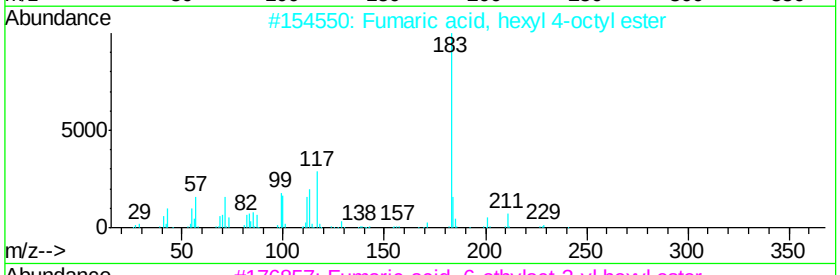
Peak Number 3 Hexadecanoic acid, 2,3-bis(... Concentration Rank 1

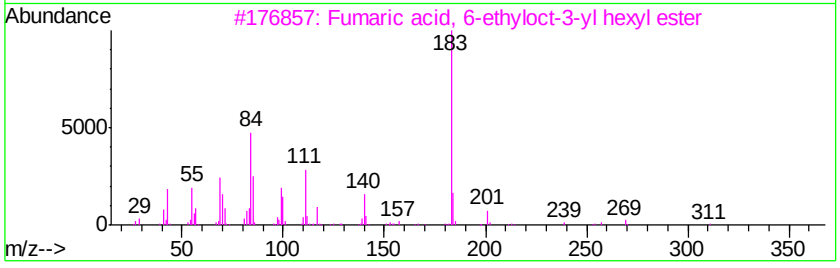
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	4.49 ng/ul	321069	Chrysene-d12	21.09

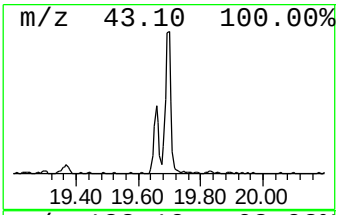
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	52
2	Fumaric acid, hexyl 4-octyl ester	312	C18H32O4	1000339-21-7	27
3	Fumaric acid, 6-ethyloct-3-yl he...	340	C20H36O4	1000339-15-3	27
4	1-Methyl-2-formylindole	159	C10H9NO	027421-51-8	18
5	Lauric anhydride	382	C24H46O3	000645-66-9	14

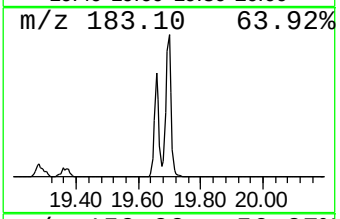


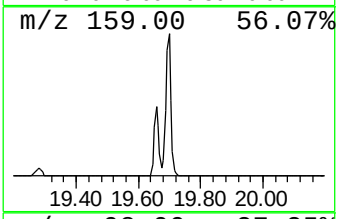


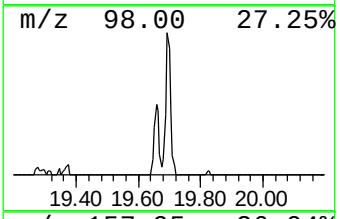


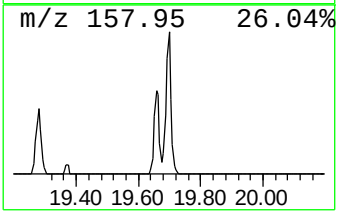












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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

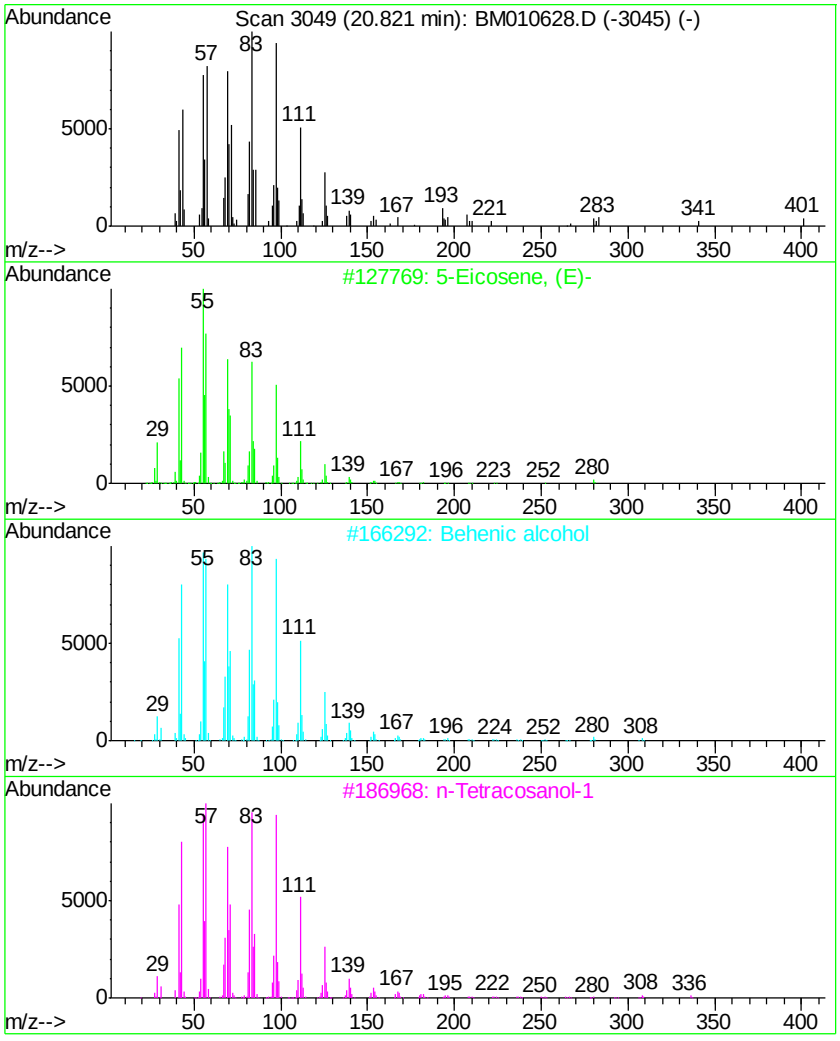
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

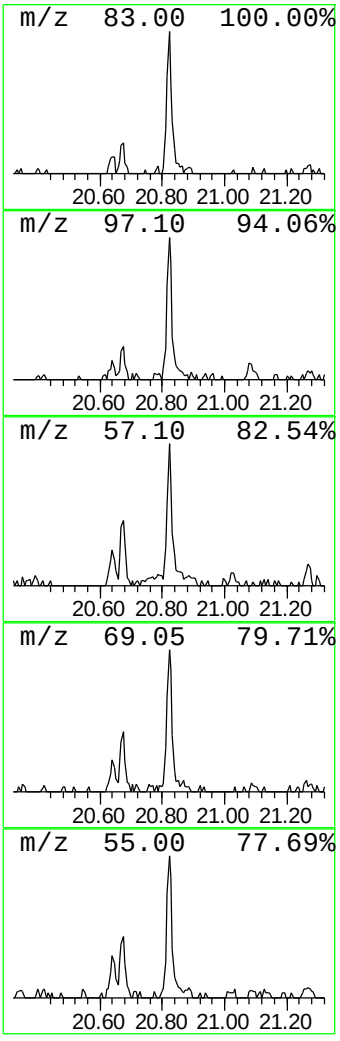
****

Peak Number 5 (DEL) Alkane: Cyclic20.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	2.15 ng/ul	154049	Chrysene-d12	21.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.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
n-Hexadecanoic acid	17.79	4.1	ng/ul	218530	4	16.87	1077320	20.0
unknown-01	19.66	2.4	ng/ul	168649	5	21.09	1430240	20.0
Hexadecanoic acid...	19.70	4.5	ng/ul	321069	5	21.09	1430240	20.0
(DEL) Alkane: Cyc...	20.82	2.1	ng/ul	154049	5	21.09	1430240	20.0