LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

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\SOM02.2-EPA-BM013017.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	3.375	130	134	141	rVB4	19882	26584	1.57%	0.106%
2	7.063	754	761	772	rBV2	375227	700750	41.30%	2.805%
3	7.245	786	792	799	rBV	246181	365948	21.57%	1.465%
4	7.445	819	826	832	rBV	372167	590868	34.82%	2.365%
5	7.916	900	906	912	rBV2	328866	541742	31.93%	2.169%
6	8.610	1018	1024	1033	rVB2	374637	610246	35.97%	2.443%
7	9.080	1097	1104	1113	rVB2	387242	626878	36.95%	2.509%
8	9.445	1160	1166	1172	rBV	12739	17773	1.05%	0.071%
9	9.798	1219	1226	1233	rBV2	340785	565124	33.31%	2.262%
10	10.004	1255	1261	1267	rBV2	40504	70511	4.16%	0.282%
11	10.327	1308	1316	1326	rBV	440935	720821	42.48%	2.886%
12	10.716	1376	1382	1390	rVB	376806	655802	38.65%	2.625%
13	10.857	1397	1406	1416	rBV	371790	645160	38.02%	2.583%
14	12.804	1733	1737	1742	rBV2	35037	49461	2.92%	0.198%
15	13.957	1927	1933	1937	rBV	741652	978173	57.65%	3.916%
16	14.004	1937	1941	1947	rVB	278100	369510	21.78%	1.479%
17	14.251	1974	1983	1991	rBV	676283	994402	58.61%	3.981%
18	14.427	2007	2013	2019	rBV6	16908	25191	1.48%	0.101%
19	14.551	2028	2034	2041	rVB	540421	798733	47.07%	3.197%
20	14.739	2059	2066	2075	rBV	406673	597191	35.20%	2.391%
21	14.951	2094	2102	2115	rBV3	215130	301706	17.78%	1.208%
22	15.333	2163	2167	2171	rBV2	22425	28672	1.69%	0.115%
23	15.380	2171	2175	2179	rVB2	40704	50819	3.00%	0.203%
24	15.545	2197	2203	2213	rVB	886101	1218394	71.81%	4.877%
25	15.656	2217	2222	2234	rVB2	374277	521112	30.71%	2.086%
26	15.780	2236	2243	2248	rBV6	21531	38415	2.26%	0.154%
27	16.239	2317	2321	2330	rBV2	52582	91125	5.37%	0.365%
28	16.680	2392	2396	2403	rVB2	57041	73556	4.34%	0.294%
29	17.033	2447	2456	2460	rBV2	59802	81768	4.82%	0.327%
30	17.086	2461	2465	2469	rVB6	18642	27375	1.61%	0.110%
31	17.298	2495	2501	2509	rBV	709807	1019912	60.11%	4.083%
32	17.398	2512	2518	2525	rVB	990816	1388599	81.84%	5.559%
33	17.774	2577	2582	2587	rBV2	57303	78973	4.65%	0.316%
34	18.056	2624	2630	2635	rBV7	9928	26426	1.56%	0.106%

LSC Area Percent Report

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Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

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\SOM02.2-EPA-BM013017.M
Title : SVOA CALIBRATION

35	18.168	2644	2649	2655	rBV	211548	271467	16.00%	1.087%
36	18.462	2696	2699	2706	rBV4	37535	64679	3.81%	0.259%
37	18.921	2773	2777	2780	rVB5	27231	29577	1.74%	0.118%
38	19.097	2803	2807	2812	rVB6	13592	18878	1.11%	0.076%
39	19.321	2839	2845	2849	rBV5	21435	34258	2.02%	0.137%
40	19.444	2861	2866	2872	rBV2	164262	218732	12.89%	0.876%
41	19.580	2884	2889	2894	rVB8	8692	19986	1.18%	0.080%
42	19.686	2899	2907	2918	rVV	1224018	1679134	98.96%	6.722%
43	19.997	2955	2960	2963	rBV	621783	645383	38.04%	2.584%
44	20.033	2963	2966	2973	rVB	954468	1058629	62.39%	4.238%
45	20.968	3121	3125	3128	rBV	313625	333151	19.63%	1.334%
46	21.003	3128	3131	3135	rVB	450791	470849	27.75%	1.885%
47	21.156	3153	3157	3165	rBV4	152799	223241	13.16%	0.894%
48	21.468	3205	3210	3215	rBV	1052662	1305498	76.94%	5.226%
49	21.850	3271	3275	3277	rBV2	130772	155401	9.16%	0.622%
50	21.880	3277	3280	3285	rVB	232448	257047	15.15%	1.029%
51	22.821	3436	3440	3443	rBV3	117487	153507	9.05%	0.615%
52	22.856	3443	3446	3453	rVB3	186192	269133	15.86%	1.077%
53	23.668	3578	3584	3596	rVB2	850382	1696738	100.00%	6.792%
54	23.821	3604	3610	3618	rVB	575450	1177738	69.41%	4.715%

Sum of corrected areas: 24980746

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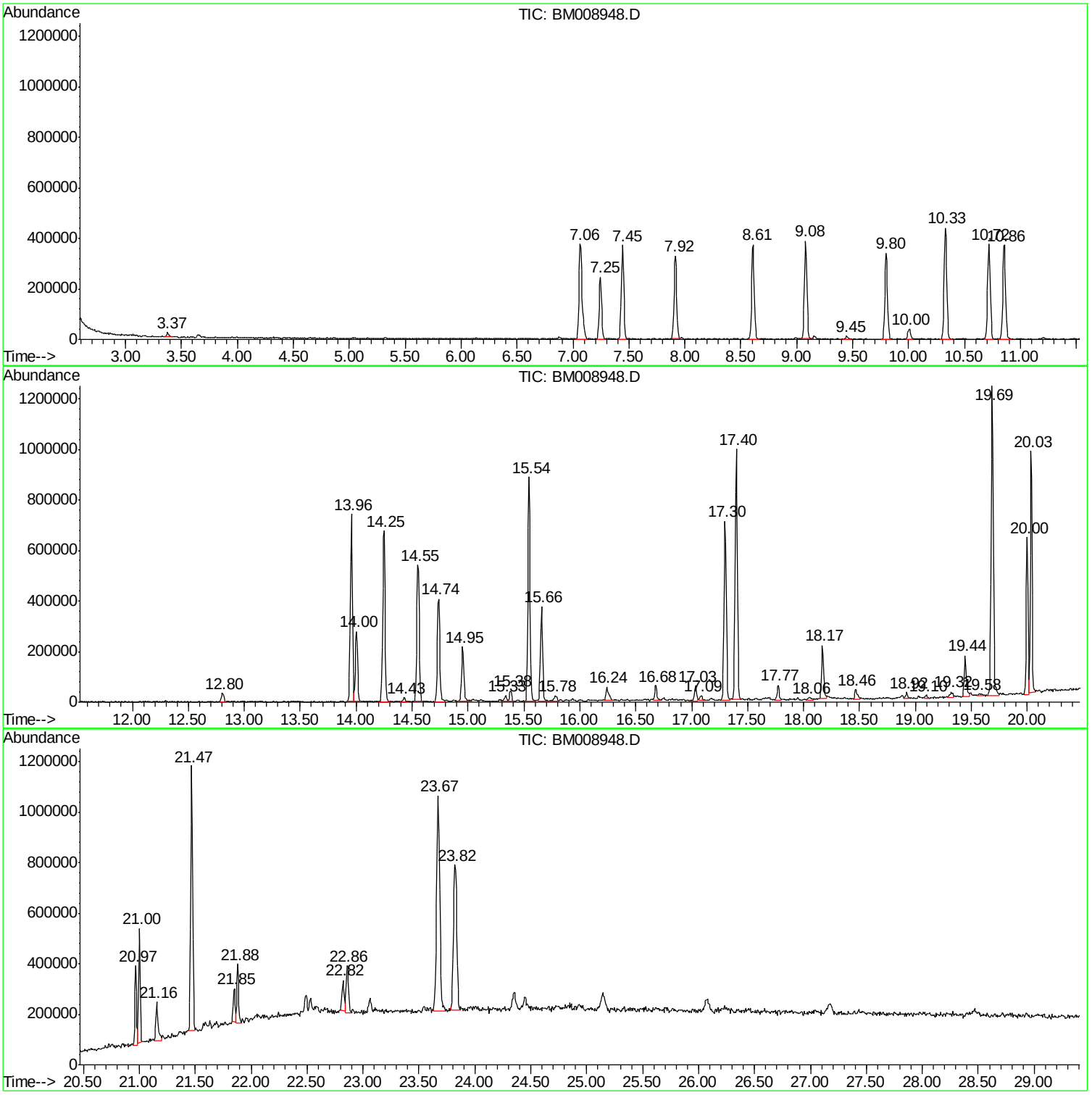
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
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Instrument : BNA_M
ClientSampleId : BDNT2

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Quant Title : SVOA CALIBRATION

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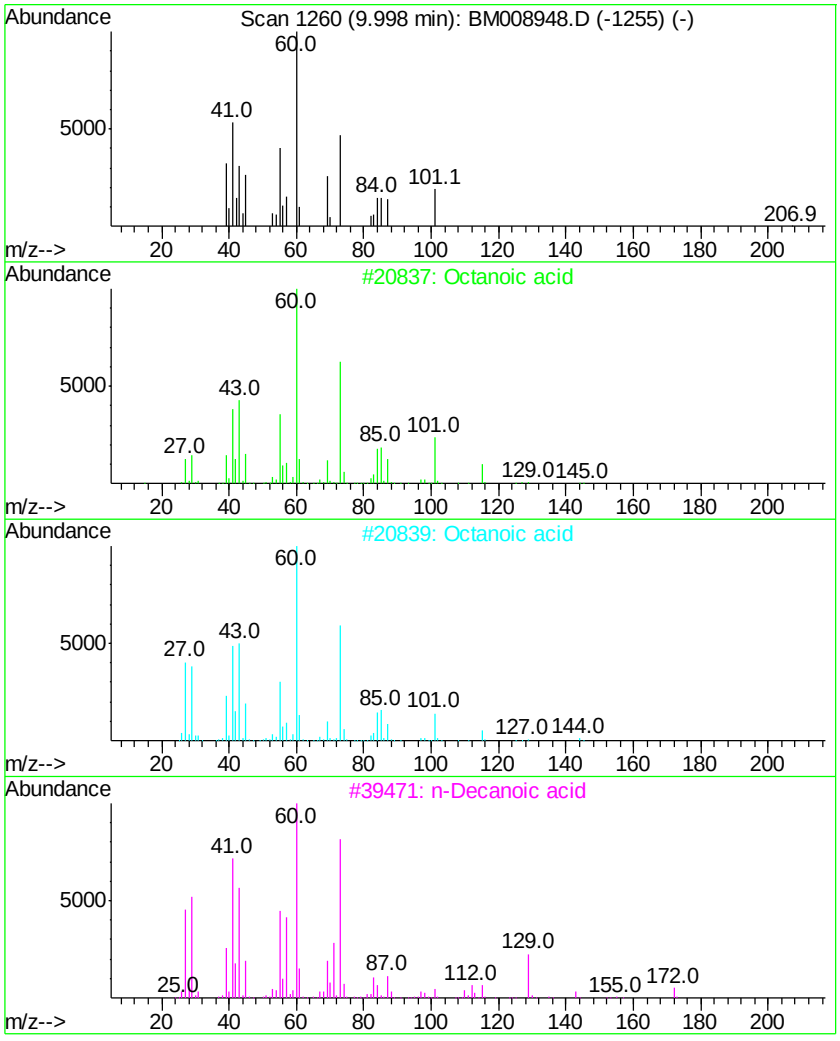
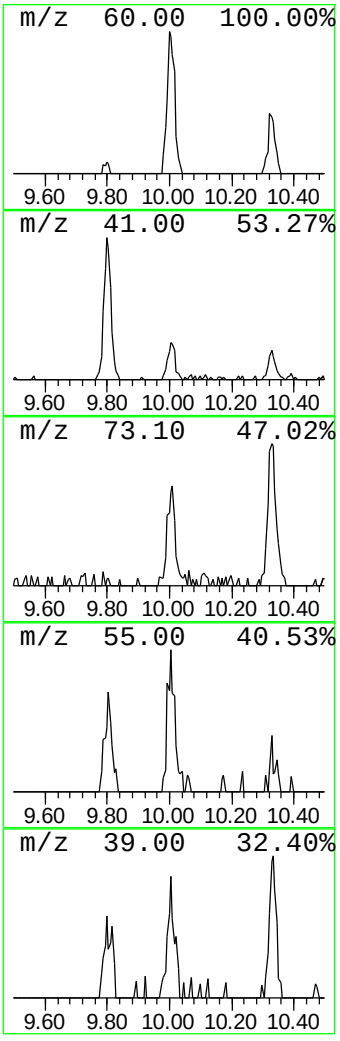
****

Peak Number 1 Octanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.00	2.15 ng/ul	70511	Naphthalene-d8	10.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	59
2	Octanoic acid	144	C8H16O2	000124-07-2	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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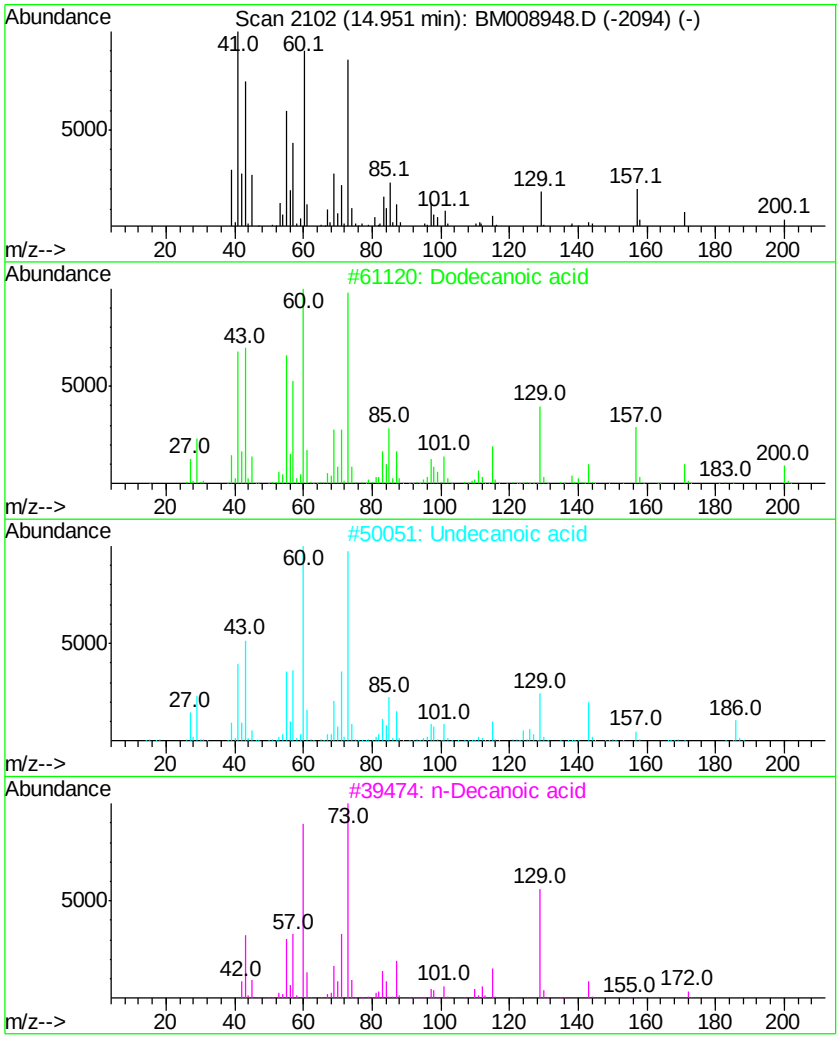
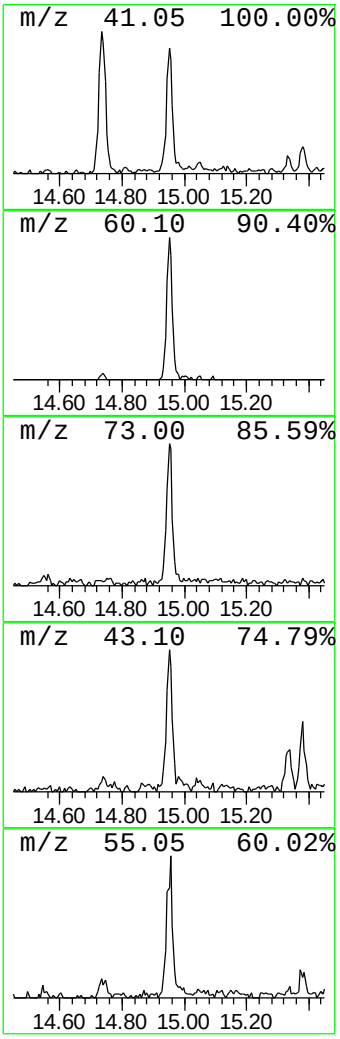
Peak Number 2 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	7.55 ng/ul	301706	Acenaphthene-d10	14.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	80
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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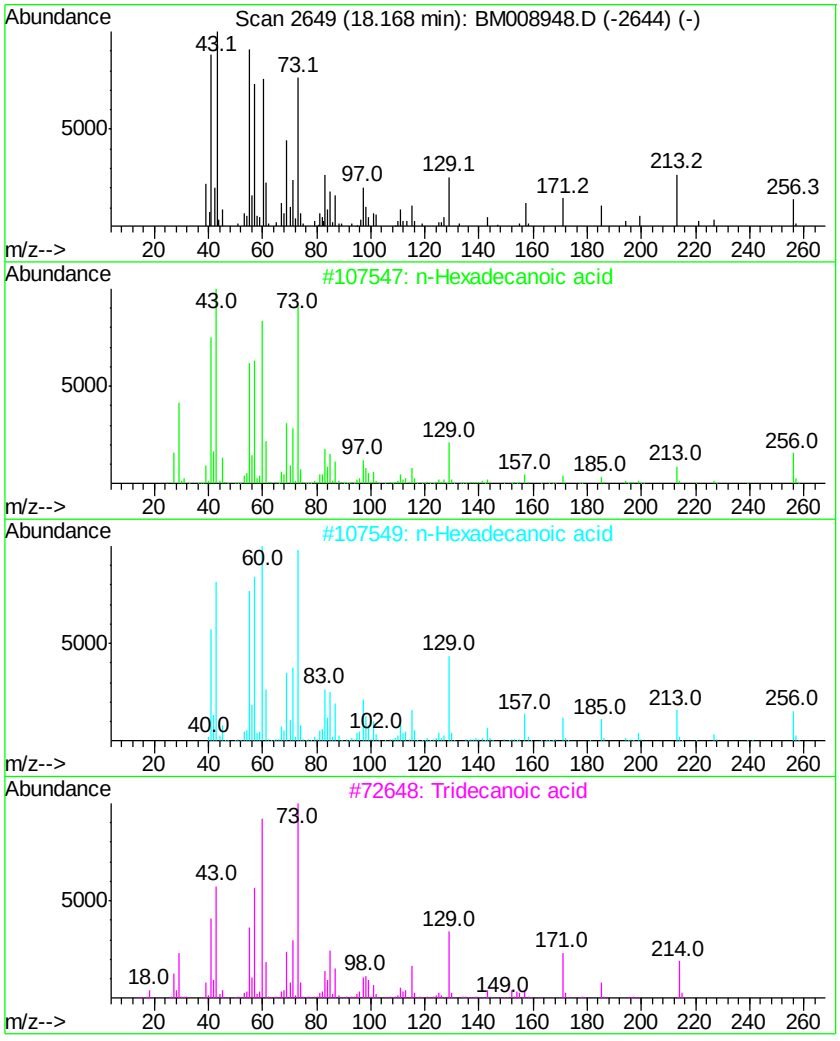
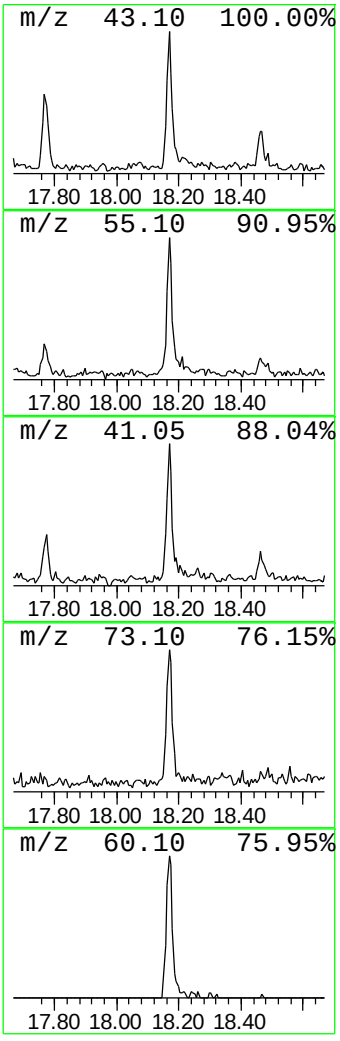
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	5.32 ng/ul	271467	Phenanthrene-d10	17.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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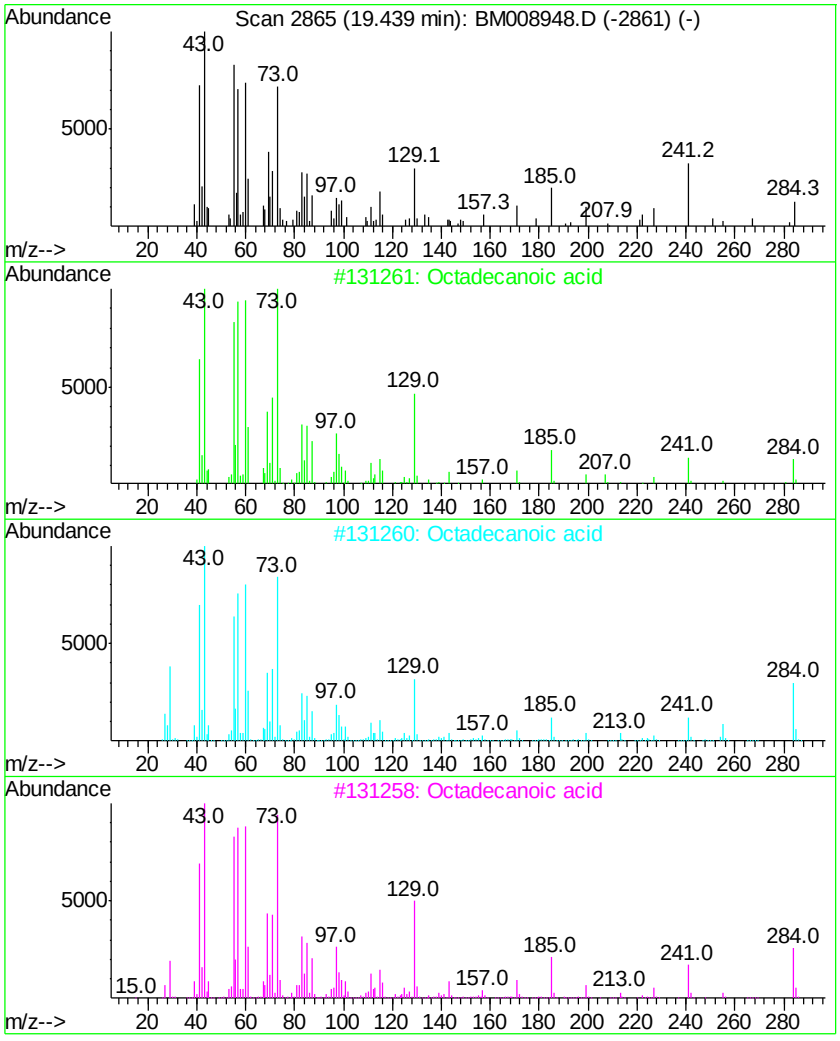
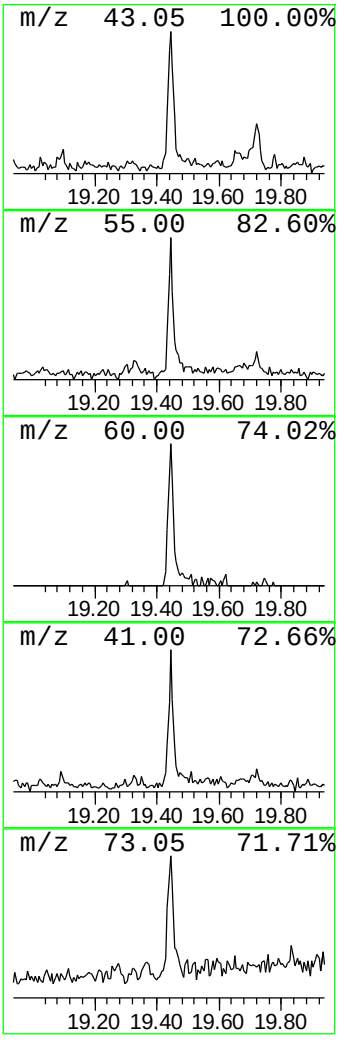
Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.44	3.35 ng/ul	218732	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Octadecanoic acid	284	C18H36O2	000057-11-4	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





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Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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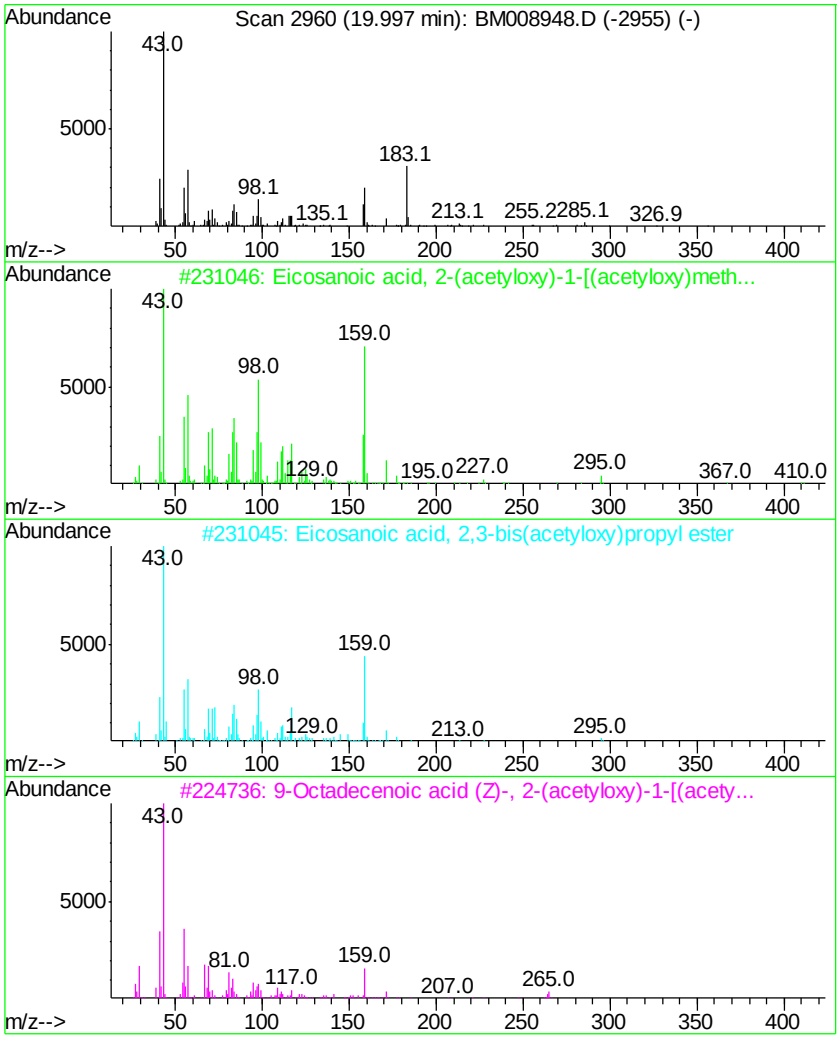
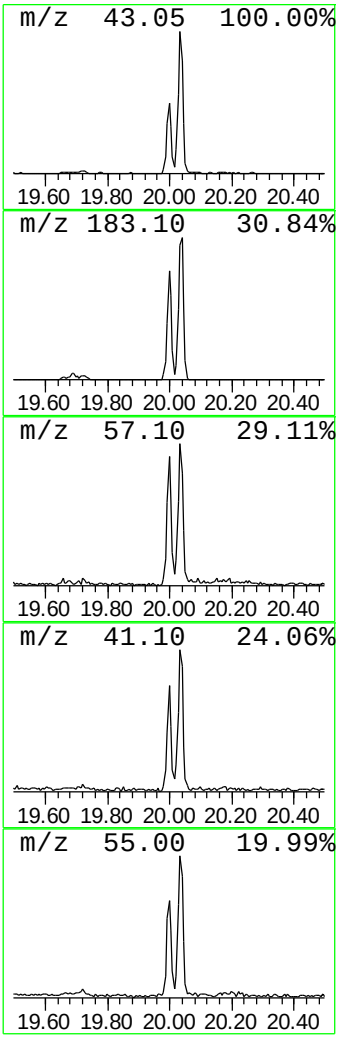
Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.00	9.89 ng/ul	645383	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	46
2	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	38
3	9-Octadecenoic acid (Z)-, 2-(ace...	440	C25H44O6	055401-63-3	23
4	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	23
5	Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	14





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ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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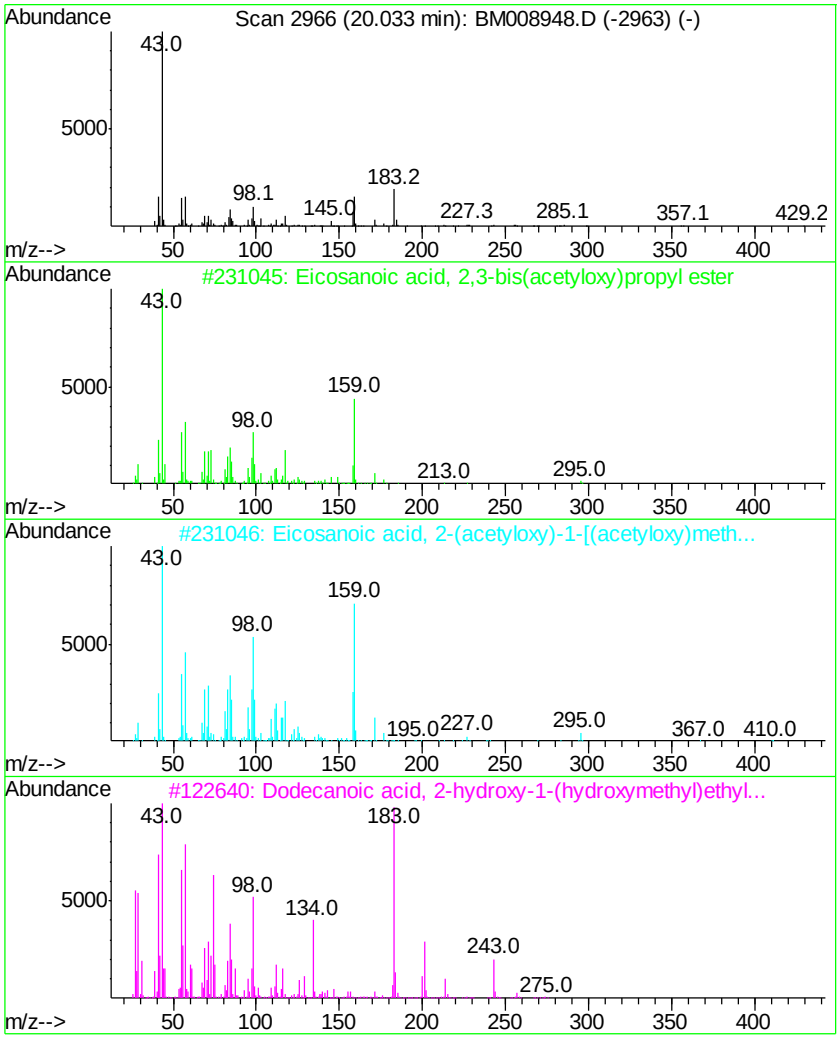
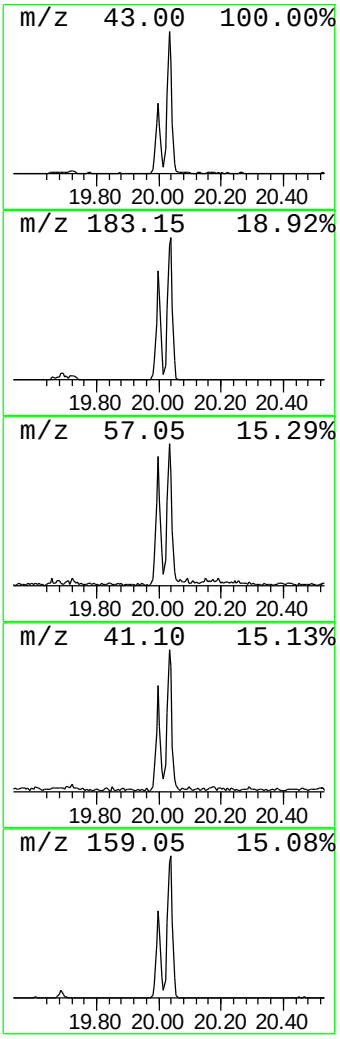
Peak Number 6 Eicosanoic acid, 2,3-bis(ac... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.03	16.22 ng/ul	1058630	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	53
2	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	47
3	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	38
4	9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	32
5	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-02-0	23





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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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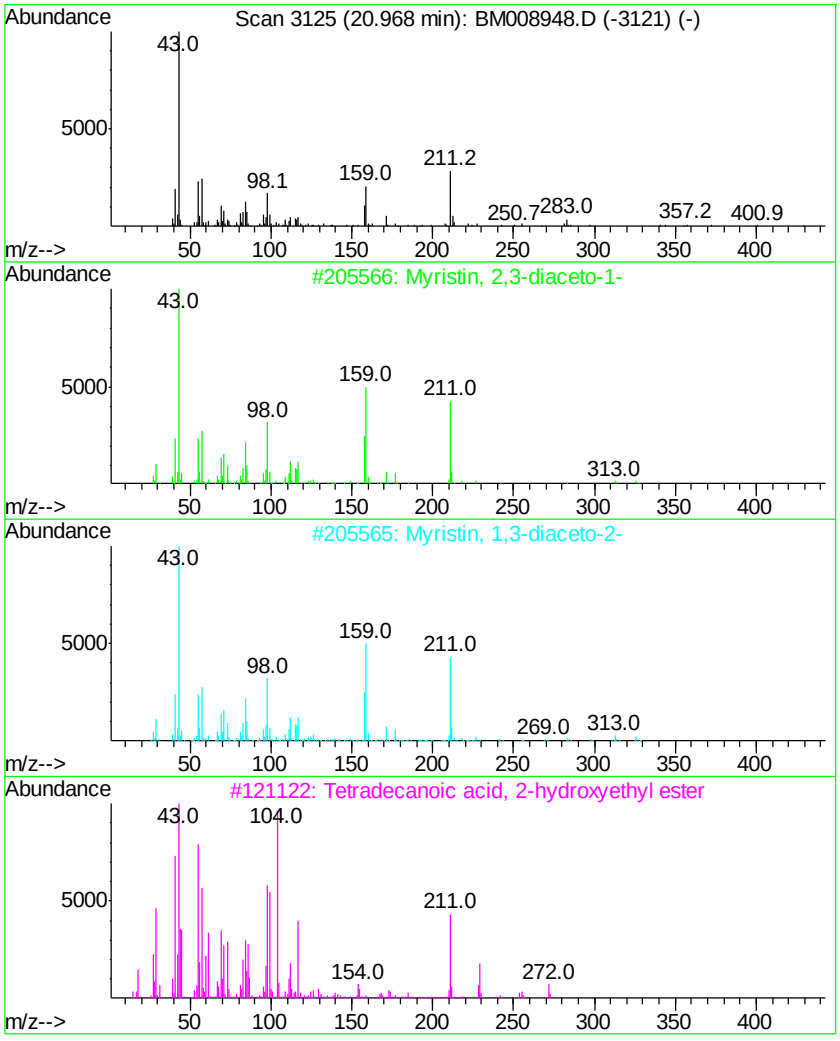
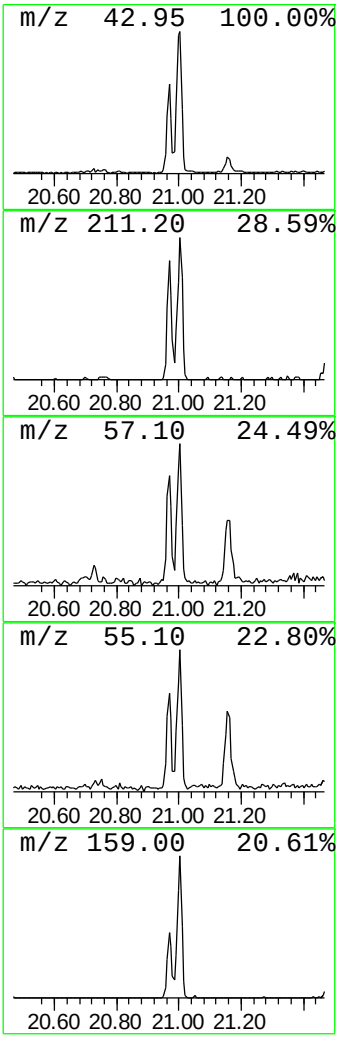
Peak Number 7 Myristin, 2,3-diaceto-1- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	5.10 ng/ul	333151	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	64
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	64
3	Tetradecanoic acid, 2-hydroxyeth...	272	C16H32O3	022122-18-5	38
4	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	32
5	Tetradecanoic acid, 2,3-dihydrox...	302	C17H34O4	000589-68-4	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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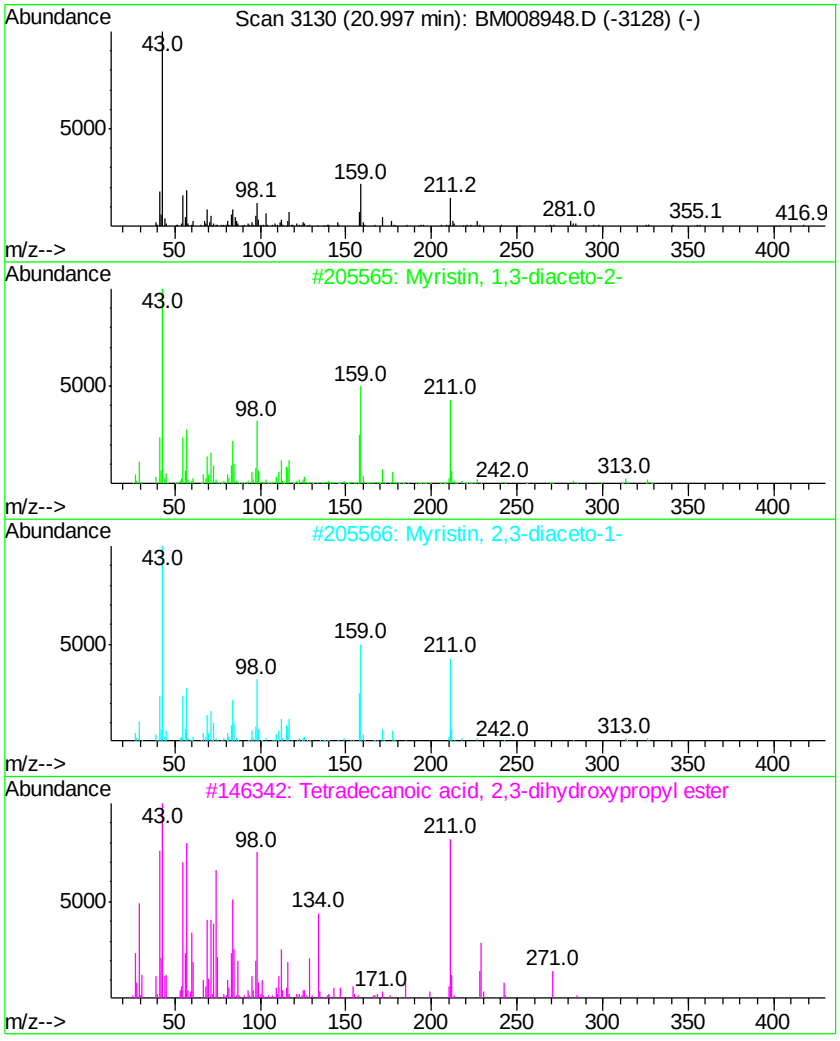
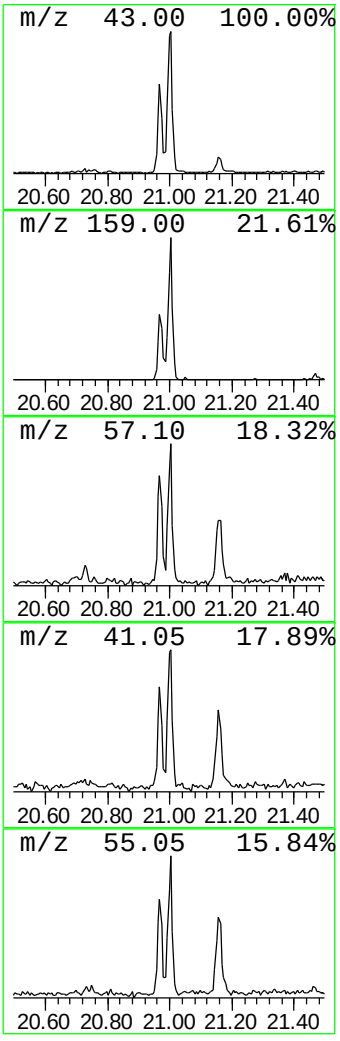
Peak Number 8 Myristin, 1,3-diaceto-2- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	7.21 ng/ul	470849	Chrysene-d12	21.47

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	68
3	Tetradecanoic acid, 2,3-dihydrox...	302	C17H34O4	000589-68-4	27
4	Tetradecanoic acid, 2-hydroxy-1-...	302	C17H34O4	003443-83-2	16
5	Sucrose, 1',2,3,3',4',6'-hexa-O-...	632	C26H37BO17	087591-47-7	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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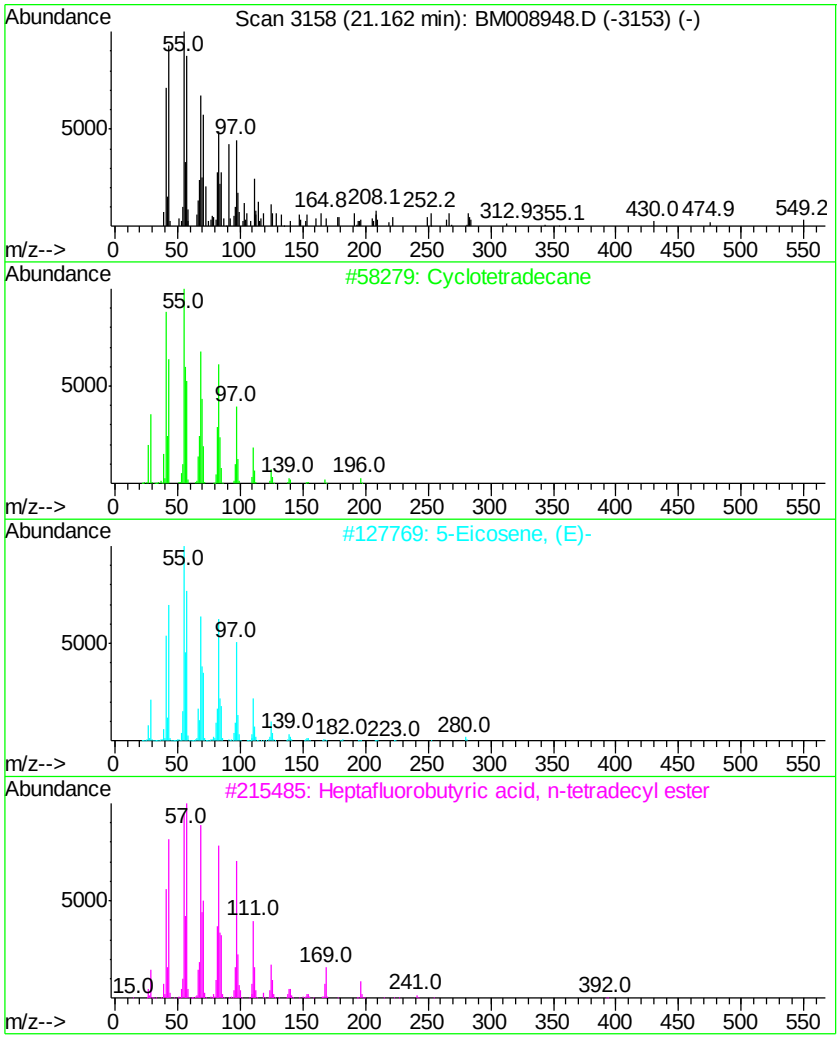
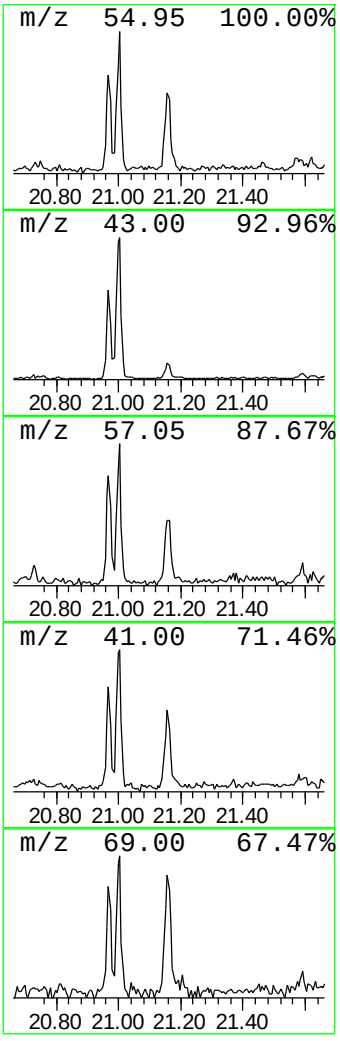
Peak Number 9 (DEL) Alkane: Cyclic21.16 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.16	3.42 ng/ul	223241	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	90
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	81
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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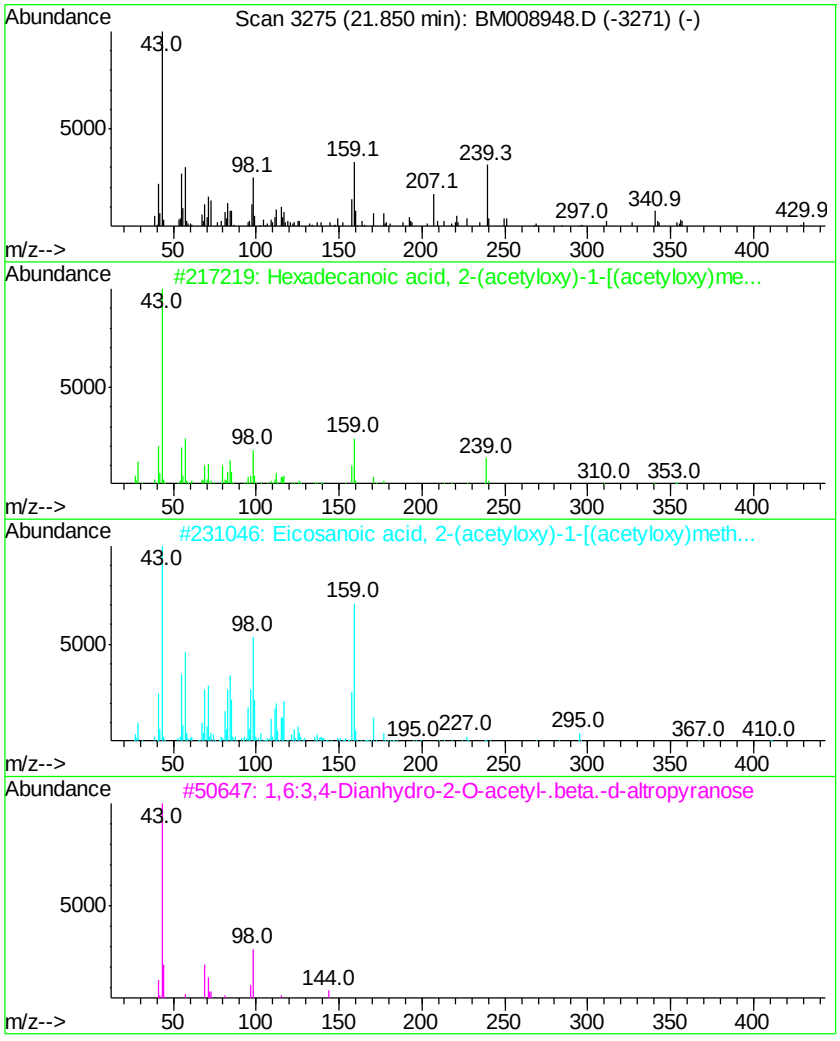
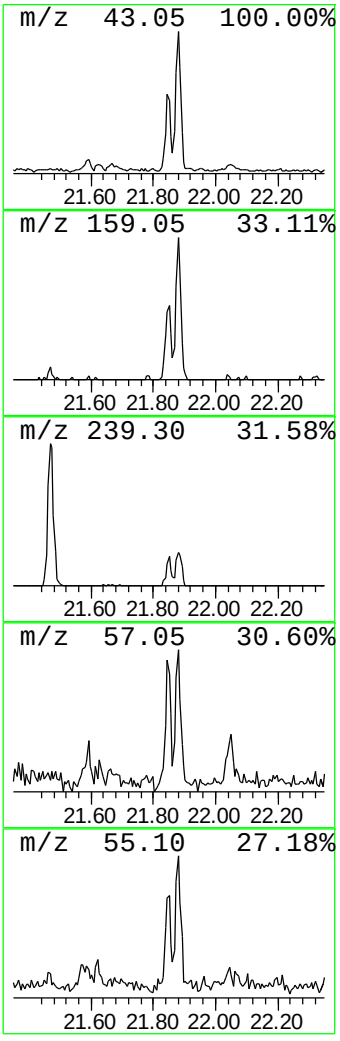
Peak Number 10 unknown-02 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.85	2.38 ng/ul	155401	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	46
2	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10
3	1,6:3,4-Dianhydro-2-O-acetyl-.be...	186	C8H10O5	1000139-89-5	10
4	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	10
5	Dodecanoyl chloride	218	C12H23ClO	000112-16-3	10





Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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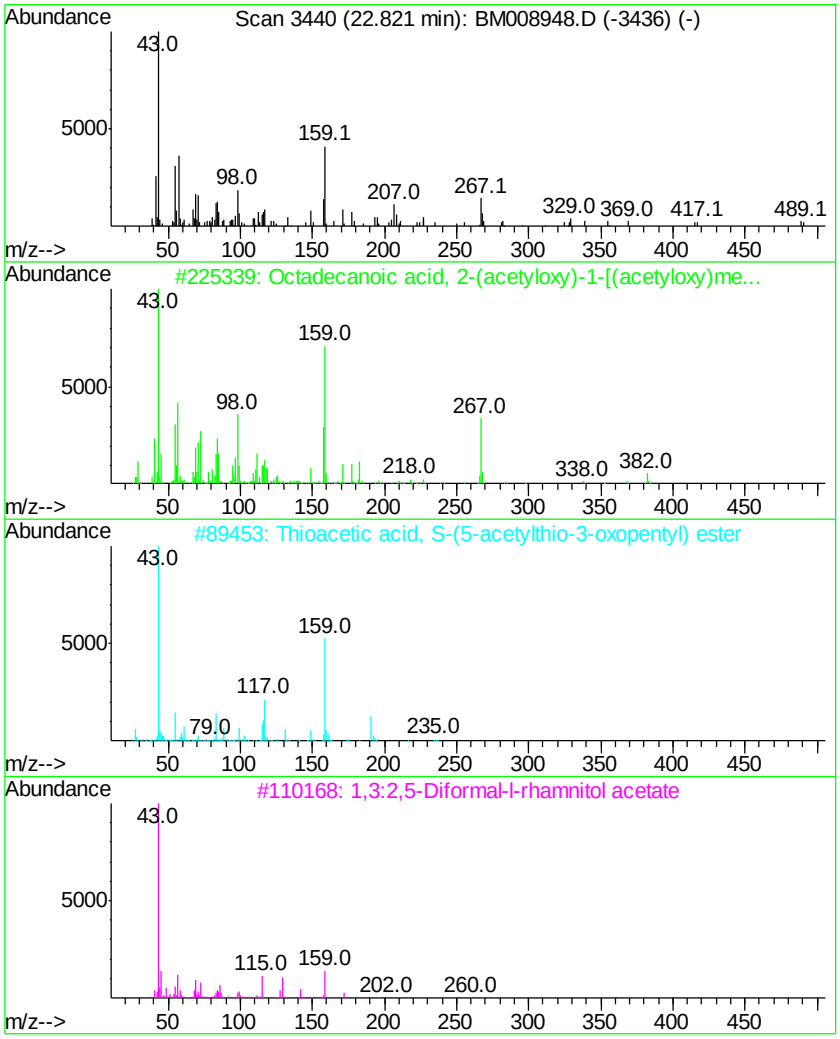
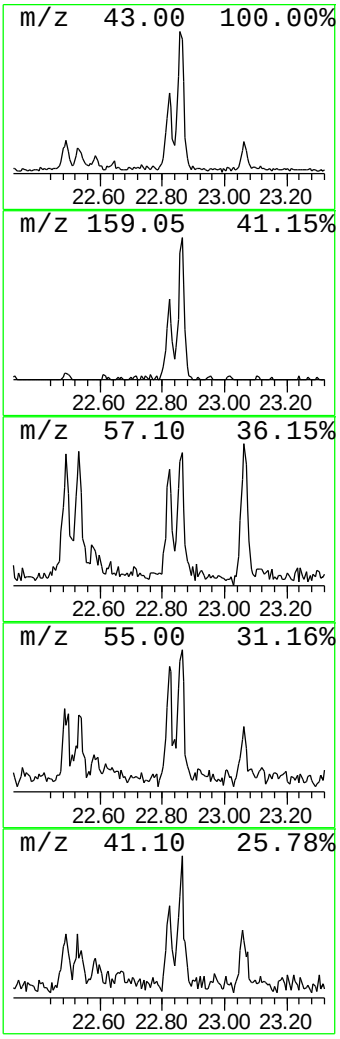
Peak Number 12 unknown-03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.82	2.61 ng/ul	153507	Perylene-d12	23.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	25
2	Thioacetic acid, S-(5-acetylthio...	234	C9H14O3S2	1000185-15-4	17
3	1,3:2,5-Diformal-l-rhamnitol ace...	260	C10H12O8	1000128-42-3	9
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	9
5	9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.M
Quant Title : SVOA CALIBRATION

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

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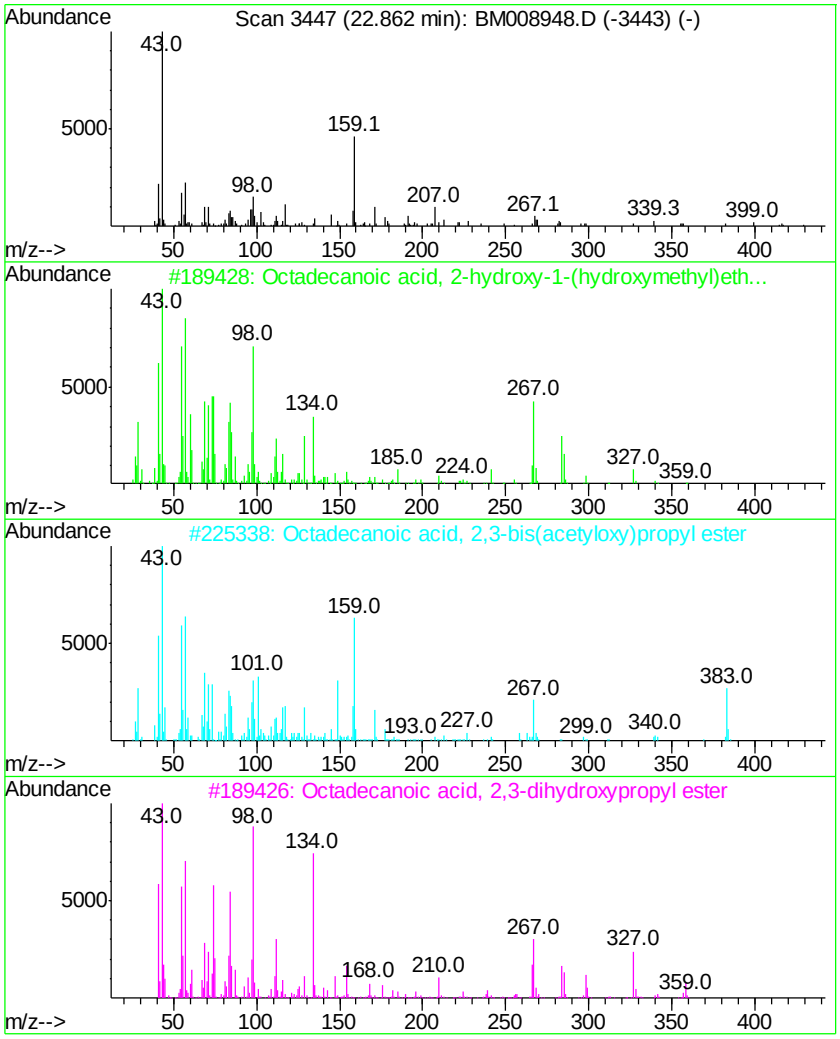
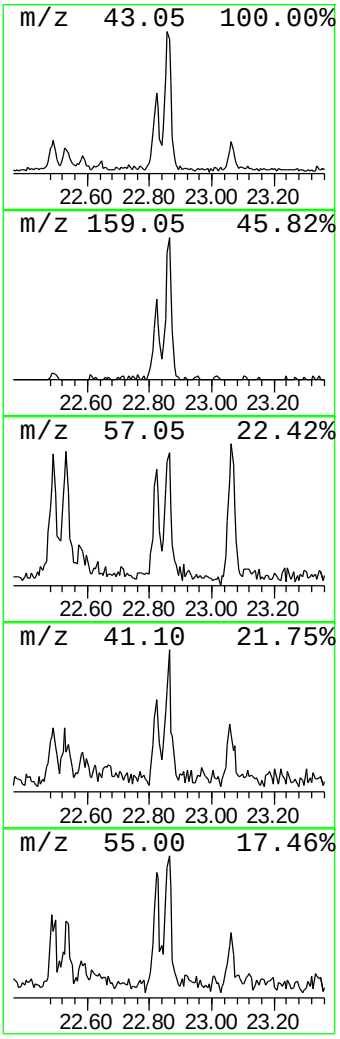
Peak Number 13 unknown-04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.86	4.57 ng/ul	269133	Perylene-d12	23.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-hydroxy-1-(...	358	C21H42O4	000621-61-4	35
2	Octadecanoic acid, 2,3-bis(acetyl...	442	C25H46O6	033599-07-4	32
3	Octadecanoic acid, 2,3-dihydroxy...	358	C21H42O4	000123-94-4	25
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	17
5	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM013117\
Data File : BM008948.D
Acq On : 31 Jan 2017 20:15
Operator : SJ/MA
Sample : I1460-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BDNT2

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM013017.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
Octanoic acid	10.00	2.1	ng/ul	70511	2	10.72	655802	20.0
Dodecanoic acid	14.95	7.5	ng/ul	301706	3	14.55	798733	20.0
n-Hexadecanoic acid	18.17	5.3	ng/ul	271467	4	17.30	1019910	20.0
Octadecanoic acid	19.44	3.4	ng/ul	218732	5	21.47	1305500	20.0
unknown-01	20.00	9.9	ng/ul	645383	5	21.47	1305500	20.0
Eicosanoic acid, ...	20.03	16.2	ng/ul	1058630	5	21.47	1305500	20.0
Myristin, 2,3-dia...	20.97	5.1	ng/ul	333151	5	21.47	1305500	20.0
Myristin, 1,3-dia...	21.00	7.2	ng/ul	470849	5	21.47	1305500	20.0
(DEL) Alkane: Cyc...	21.16	3.4	ng/ul	223241	5	21.47	1305500	20.0
unknown-02	21.85	2.4	ng/ul	155401	5	21.47	1305500	20.0
unknown-03	22.82	2.6	ng/ul	153507	6	23.83	1177740	20.0
unknown-04	22.86	4.6	ng/ul	269133	6	23.83	1177740	20.0