LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

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-BM052717.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	7.087	671	680	691	rBV2	1941970	4265877	28.24%	2.170%
2	7.245	701	707	716	rBV	1281889	1939168	12.84%	0.987%
3	7.440	734	740	749	rBV	2095939	3328619	22.04%	1.693%
4	7.904	811	819	828	rBV	2613147	4152897	27.49%	2.113%
5	8.181	858	866	871	rBV5	114829	214725	1.42%	0.109%
6	8.628	933	942	953	rBV	2086825	3394502	22.47%	1.727%
7	9.086	1012	1020	1029	rBV	1912985	3226247	21.36%	1.641%
8	9.798	1134	1141	1154	rBV	1824332	3082188	20.40%	1.568%
9	9.975	1162	1171	1179	rBV	104673	252993	1.67%	0.129%
10	10.333	1224	1232	1245	rBV	2867666	4946304	32.74%	2.516%
11	10.710	1287	1296	1308	rBV	3389555	5676502	37.58%	2.888%
12	10.869	1315	1323	1337	rBV	1378876	2506865	16.60%	1.275%
13	12.451	1585	1592	1612	rBV	2255334	3798243	25.14%	1.932%
14	13.363	1742	1747	1756	rVB7	94357	179808	1.19%	0.091%
15	13.957	1840	1848	1852	rBV	5561734	7615902	50.42%	3.875%
16	14.004	1852	1856	1862	rVB	2043648	2744018	18.17%	1.396%
17	14.239	1886	1896	1904	rBV	5882610	8245688	54.59%	4.195%
18	14.539	1940	1947	1956	rBV2	5632481	8358016	55.33%	4.252%
19	14.780	1979	1988	2001	rBV	2122098	3387177	22.42%	1.723%
20	15.321	2076	2080	2083	rBV2	140313	177692	1.18%	0.090%
21	15.533	2109	2116	2123	rBV	7831863	10604927	70.20%	5.395%
22	15.657	2131	2137	2144	rBV	2676330	3560662	23.57%	1.811%
23	15.763	2151	2155	2160	rVB2	102515	152057	1.01%	0.077%
24	16.180	2221	2226	2231	rBV2	159649	231994	1.54%	0.118%
25	16.968	2354	2360	2364	rBV6	135275	206514	1.37%	0.105%
26	17.139	2385	2389	2394	rBV5	111791	177788	1.18%	0.090%
27	17.286	2407	2414	2421	rBV2	7846835	10950210	72.49%	5.571%
28	17.386	2424	2431	2442	rVV2	8758592	11856412	78.49%	6.032%
29	18.021	2532	2539	2542	rBV7	101013	229506	1.52%	0.117%
30	18.139	2552	2559	2570	rBV	2674121	3893360	25.77%	1.981%
31	18.715	2653	2657	2665	rVB8	106329	160456	1.06%	0.082%
32	19.268	2747	2751	2752	rBV	234324	263096	1.74%	0.134%
33	19.292	2752	2755	2757	rVV3	146474	184254	1.22%	0.094%
34	19.403	2770	2774	2788	rBV	1410808	2005537	13.28%	1.020%

LSC Area Percent Report

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Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

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-BM052717.M
Title : SVOA CALIBRATION

35	19.562	2796	2801	2806	rBV2	135798	254943	1.69%	0.130%
36	19.674	2814	2820	2830	rBV	11803194	15105659	100.00%	7.685%
37	20.139	2896	2899	2904	rVB	222061	259489	1.72%	0.132%
38	20.198	2906	2909	2911	rBV4	113984	162117	1.07%	0.082%
39	20.315	2915	2929	2931	rBV8	835776	2895257	19.17%	1.473%
40	20.615	2977	2980	2986	rVB2	273324	433816	2.87%	0.221%
41	21.115	3059	3065	3073	rBV2	1858208	3657452	24.21%	1.861%
42	21.415	3113	3116	3118	rBV3	399255	496781	3.29%	0.253%
43	21.450	3118	3122	3128	rVB	11102145	13971378	92.49%	7.108%
44	21.968	3207	3210	3213	rBV2	532568	779417	5.16%	0.397%
45	22.009	3213	3217	3226	rVB	1523475	2811025	18.61%	1.430%
46	22.339	3269	3273	3279	rBV4	532698	891880	5.90%	0.454%
47	22.956	3373	3378	3384	rVB	3990026	5602208	37.09%	2.850%
48	23.033	3388	3391	3403	rVB5	674299	1447760	9.58%	0.737%
49	23.533	3472	3476	3482	rVB2	823367	1457294	9.65%	0.741%
50	23.644	3488	3495	3509	rVB2	6339928	12235803	81.00%	6.225%
51	23.797	3514	3521	3529	rVB	5897301	11090396	73.42%	5.642%
52	24.197	3583	3589	3600	rVB	3772670	7036341	46.58%	3.580%

Sum of corrected areas: 196559220

LSC Report - Integrated Chromatogram

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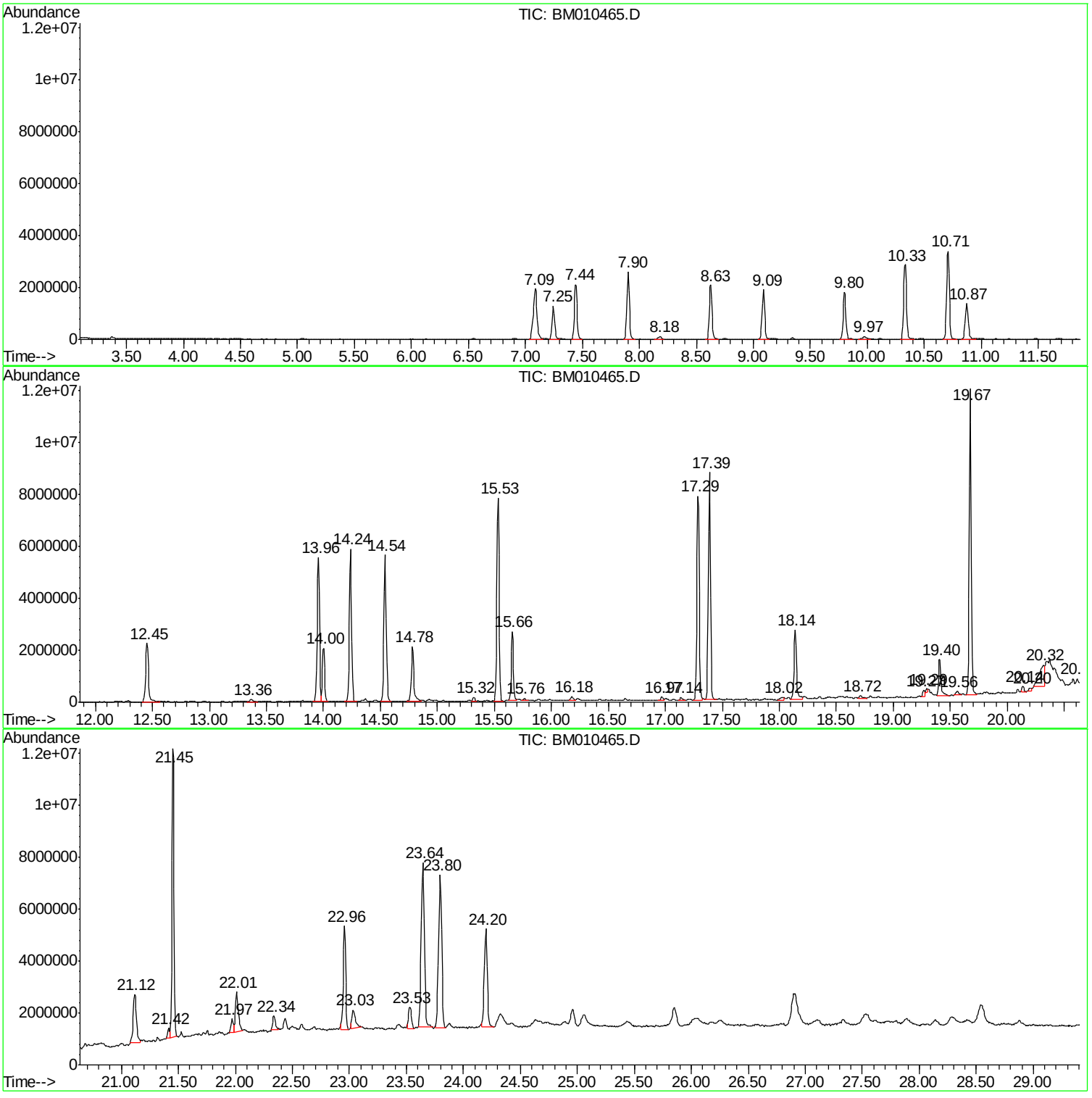
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.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\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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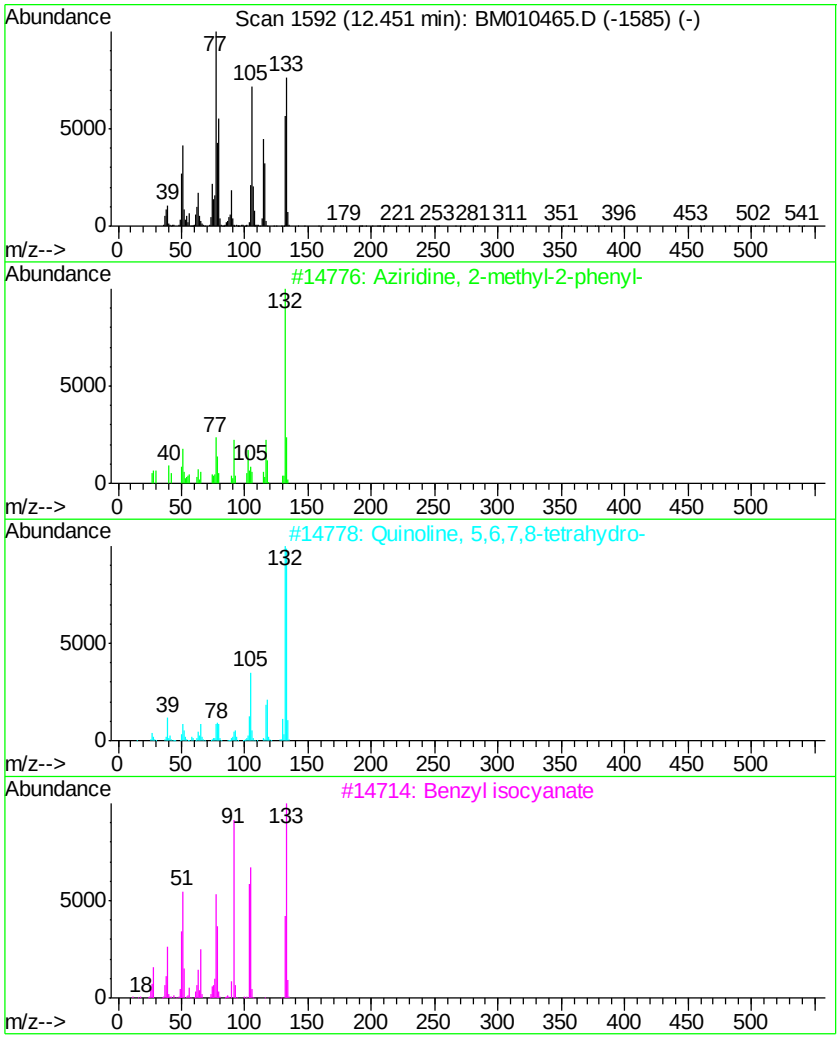
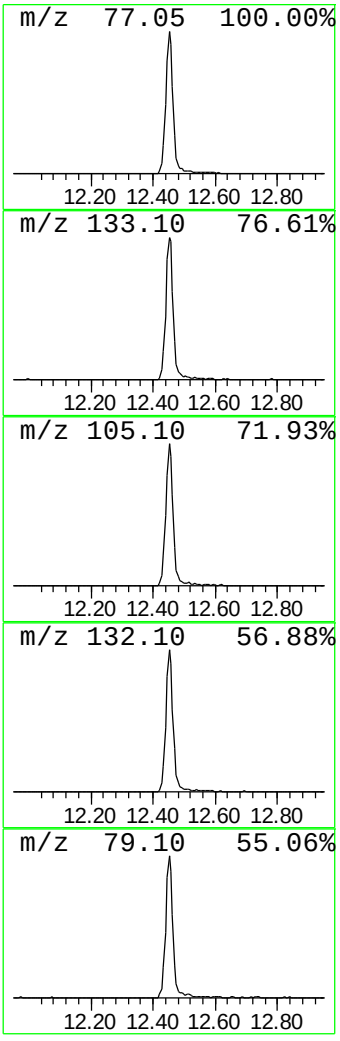
Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	13.38 ng/ul	3798240	Naphthalene-d8	10.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 2-methyl-2-phenyl-	133	C9H11N	022596-57-2	46
2	Quinoline, 5,6,7,8-tetrahydro-	133	C9H11N	010500-57-9	35
3	Benzyl isocyanate	133	C8H7NO	003173-56-6	30
4	Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	27
5	1-Aziridinecarboxamide, N-(4-met...	176	C10H12N2O	000829-65-2	25





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Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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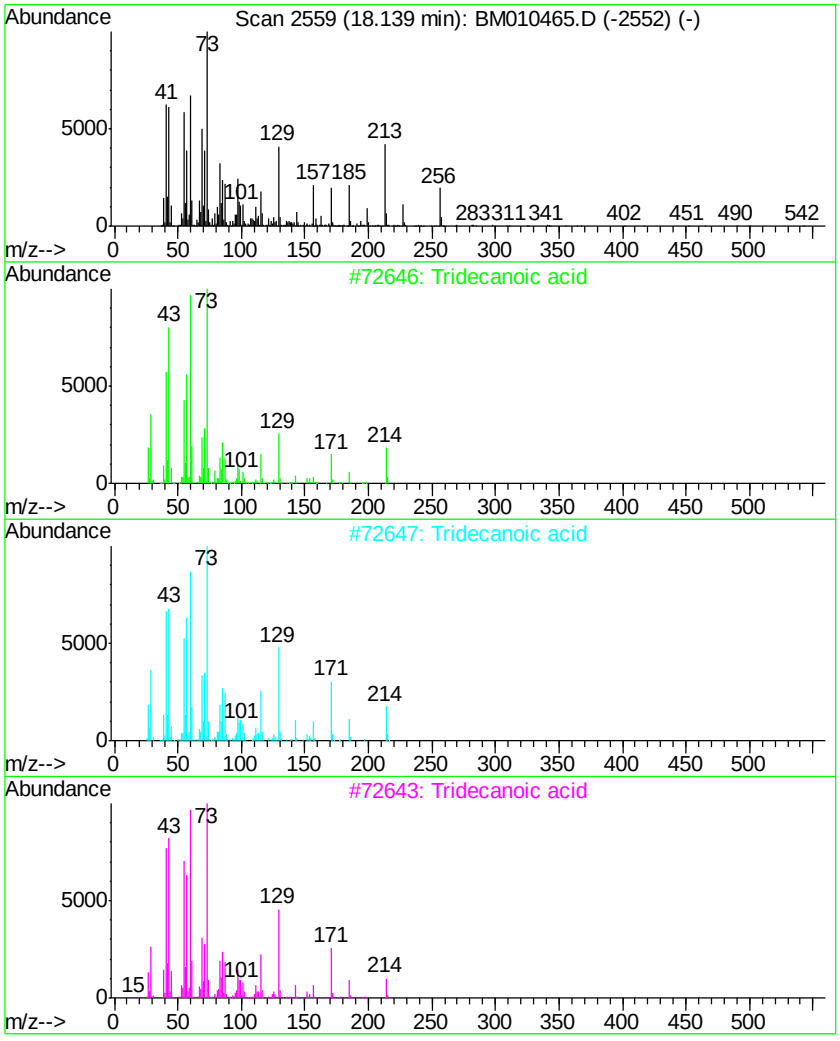
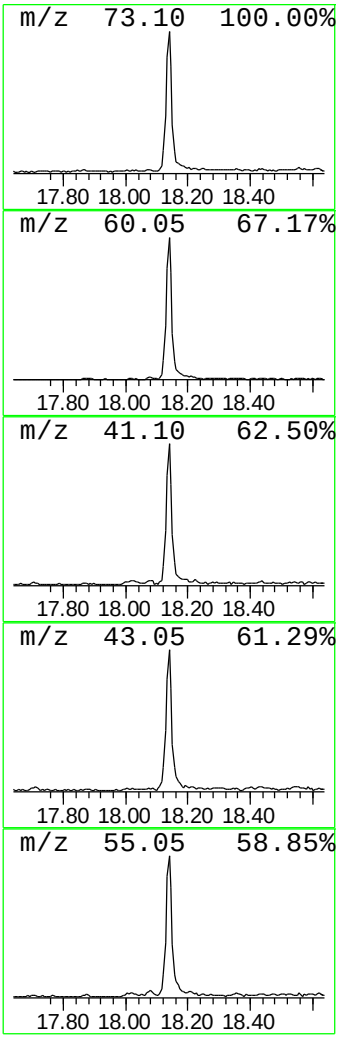
Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	7.11 ng/ul	3893360	Phenanthrene-d10	17.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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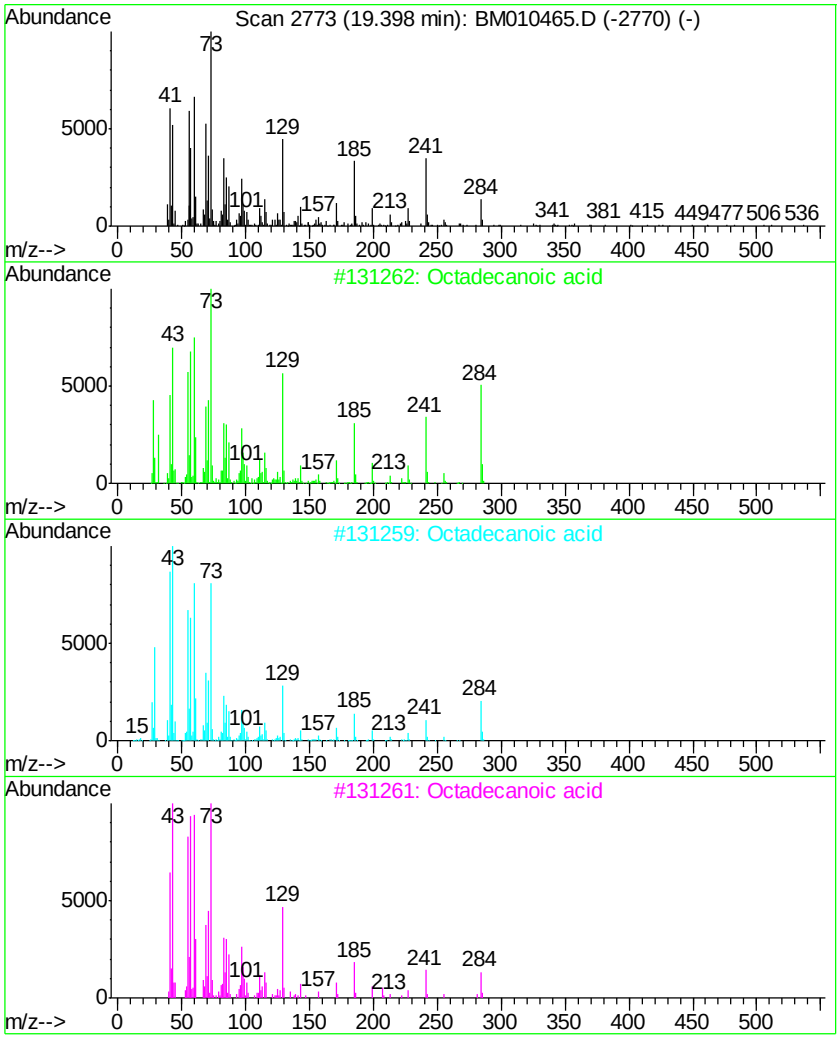
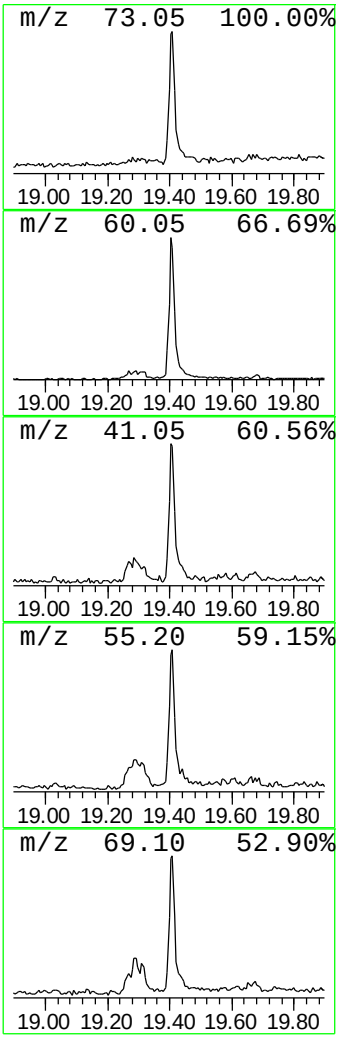
Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.40	2.87 ng/ul	2005540	Chrysene-d12	21.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	96
4	Octadecanoic acid	284	C18H36O2	000057-11-4	96
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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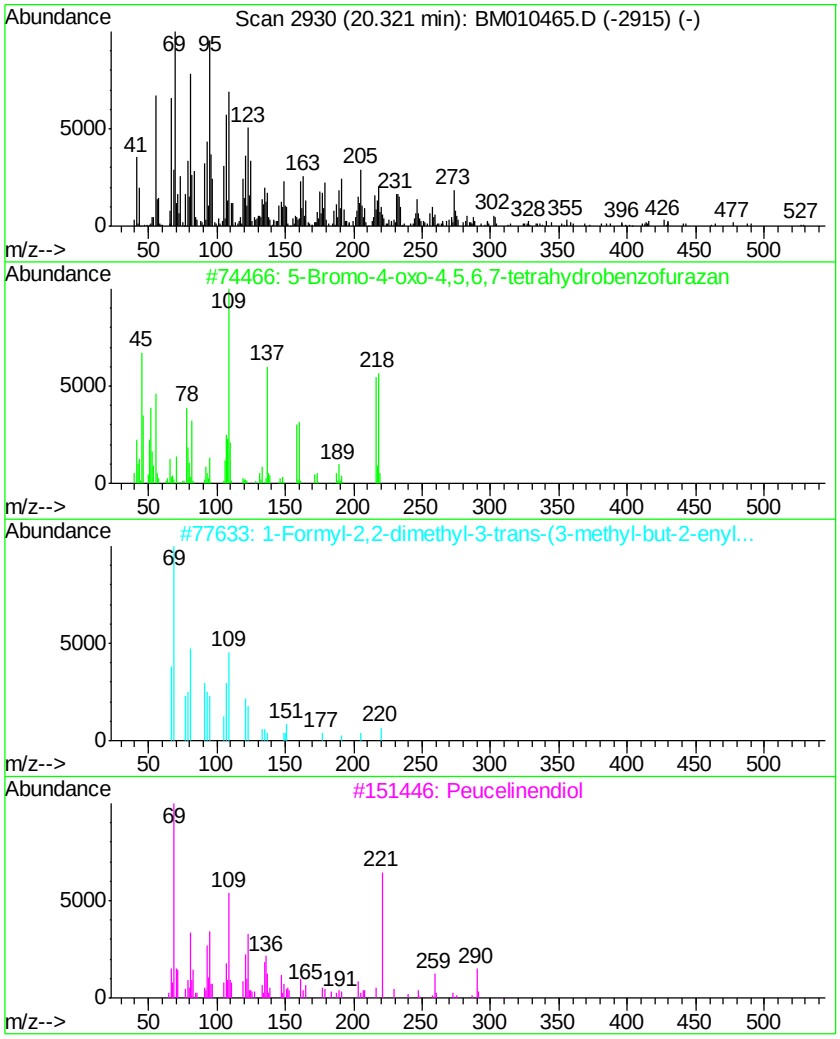
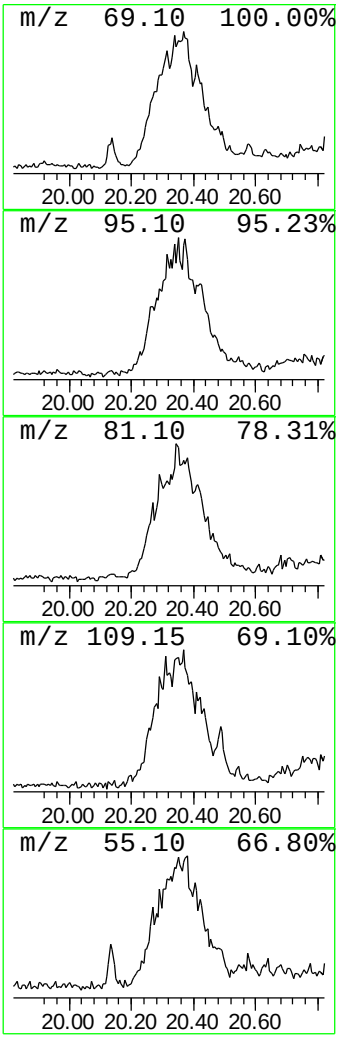
Peak Number 4 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.32	4.14 ng/ul	2895260	Chrysene-d12	21.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60
2	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	53
3	Peucelinendiol	308	C20H36O2	072776-48-8	53
4	1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	50
5	(1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy...	296	C18H32O3	1000298-98-4	49





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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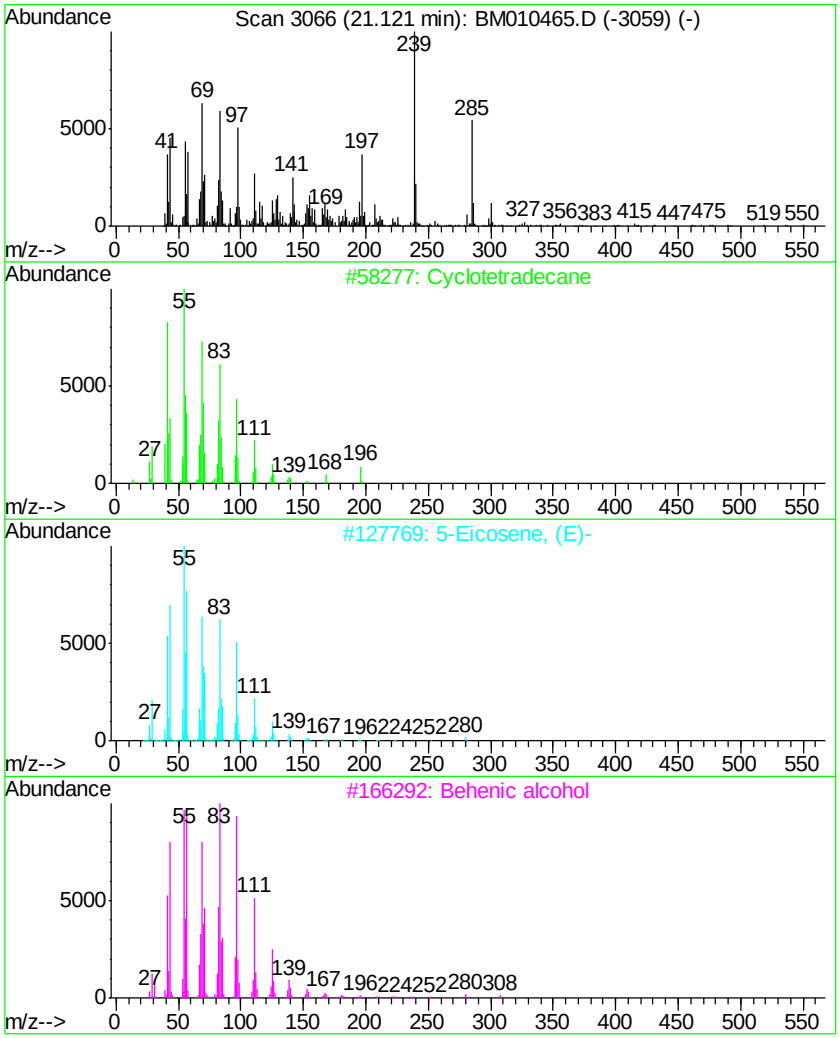
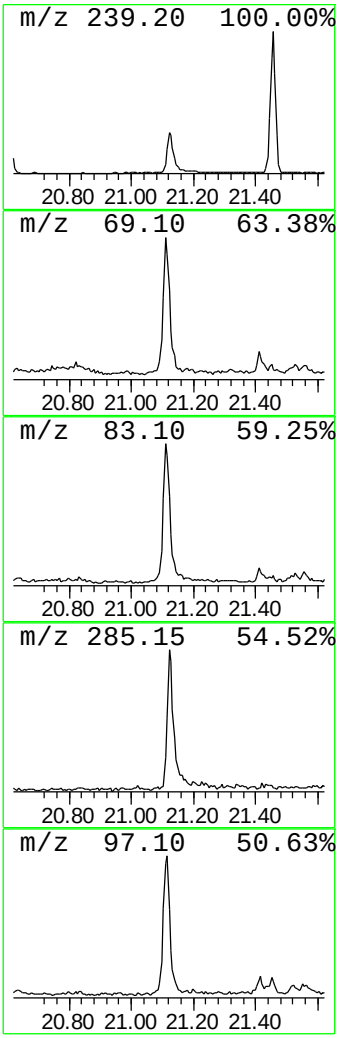
Peak Number 5 (DEL) Alkane: Cyclic21.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.12	5.24 ng/ul	3657450	Chrysene-d12	21.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	Behenic alcohol	326	C22H46O	000661-19-8	78
4	1-Heneicosanol	312	C21H44O	015594-90-8	60
5	Cyclohexadecane	224	C16H32	000295-65-8	60





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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

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

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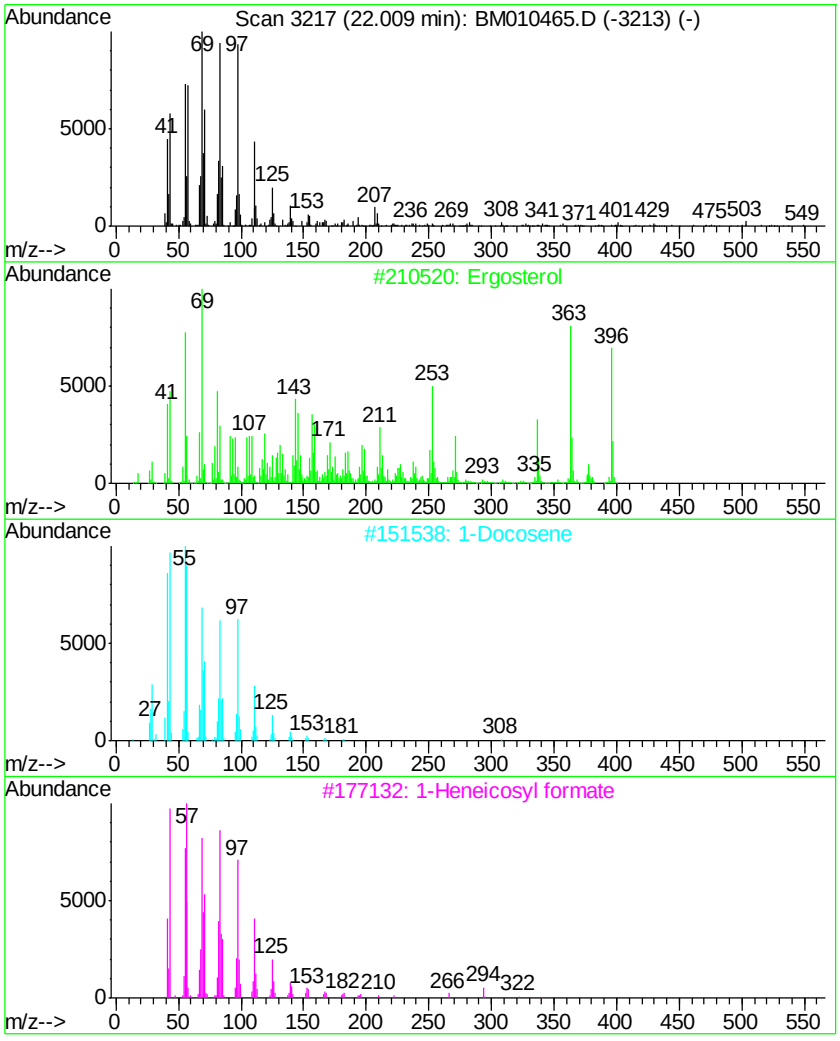
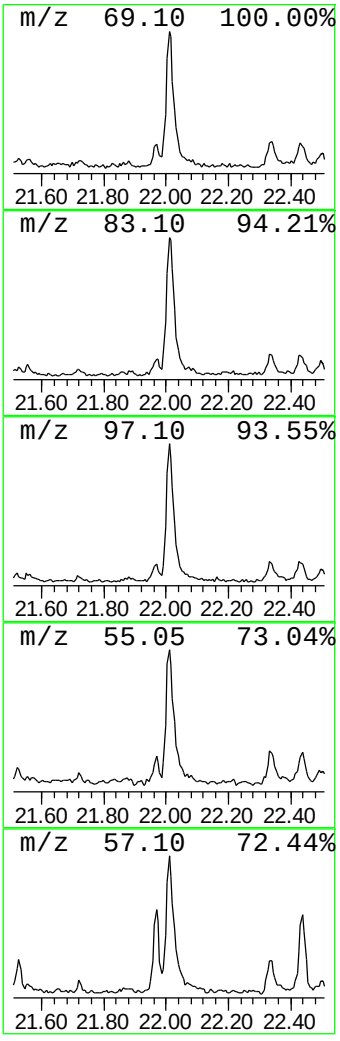
Peak Number 6 Ergosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.01	4.02 ng/ul	2811030	Chrysene-d12	21.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergosterol	396	C28H44O	000057-87-4	90
2	1-Docosene	308	C22H44	001599-67-3	89
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	81
4	1-Heneicosanol	312	C21H44O	015594-90-8	76
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	70





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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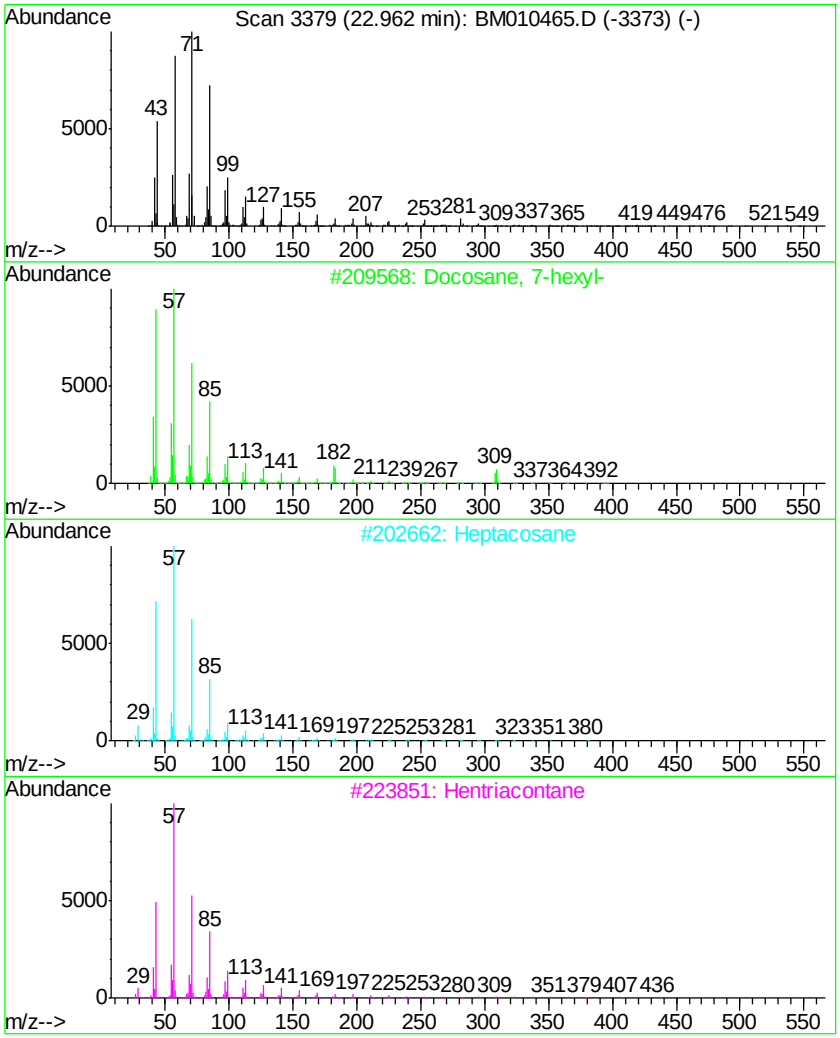
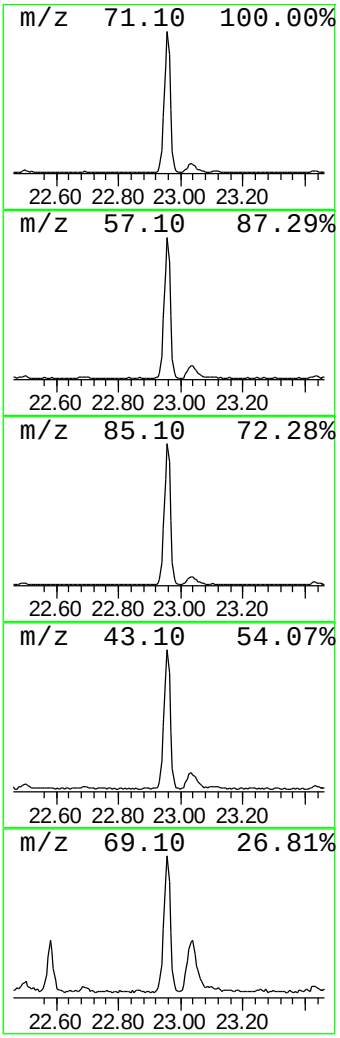
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	10.10 ng/ul	5602210	Perylene-d12	23.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	89





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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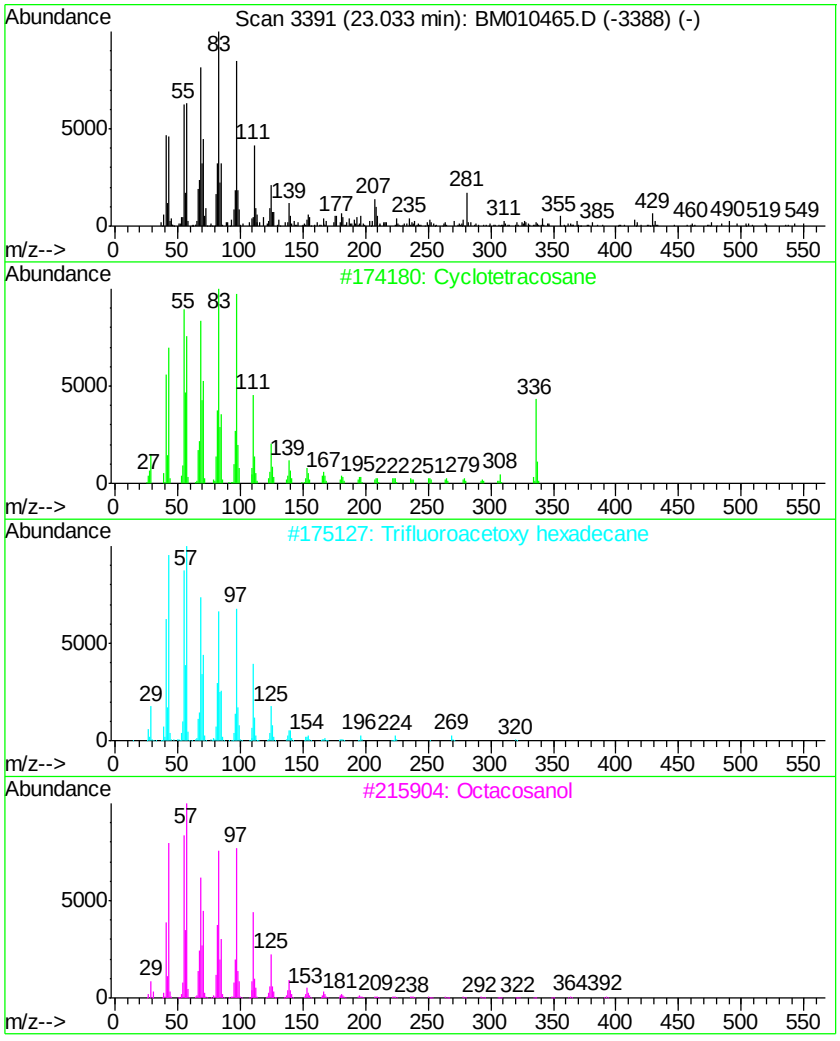
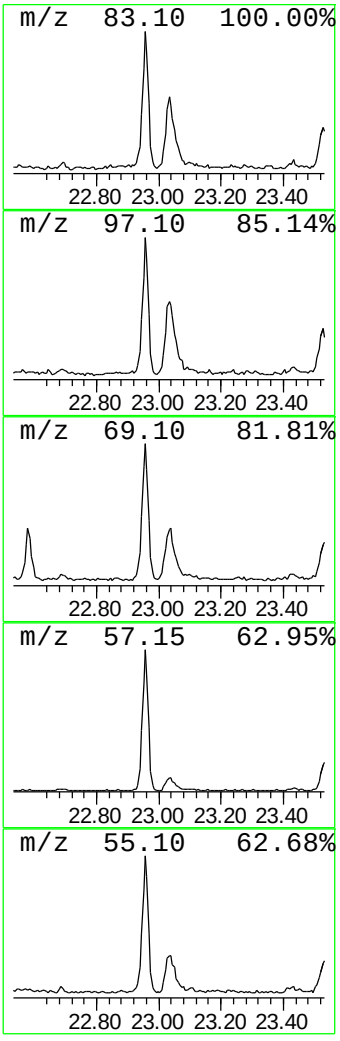
Peak Number 8 (DEL) Alkane: Cyclic23.03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.03	2.61 ng/ul	1447760	Perylene-d12	23.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	89
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
3	Octacosanol	410	C28H58O	000557-61-9	64
4	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
5	Behenic alcohol	326	C22H46O	000661-19-8	55





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Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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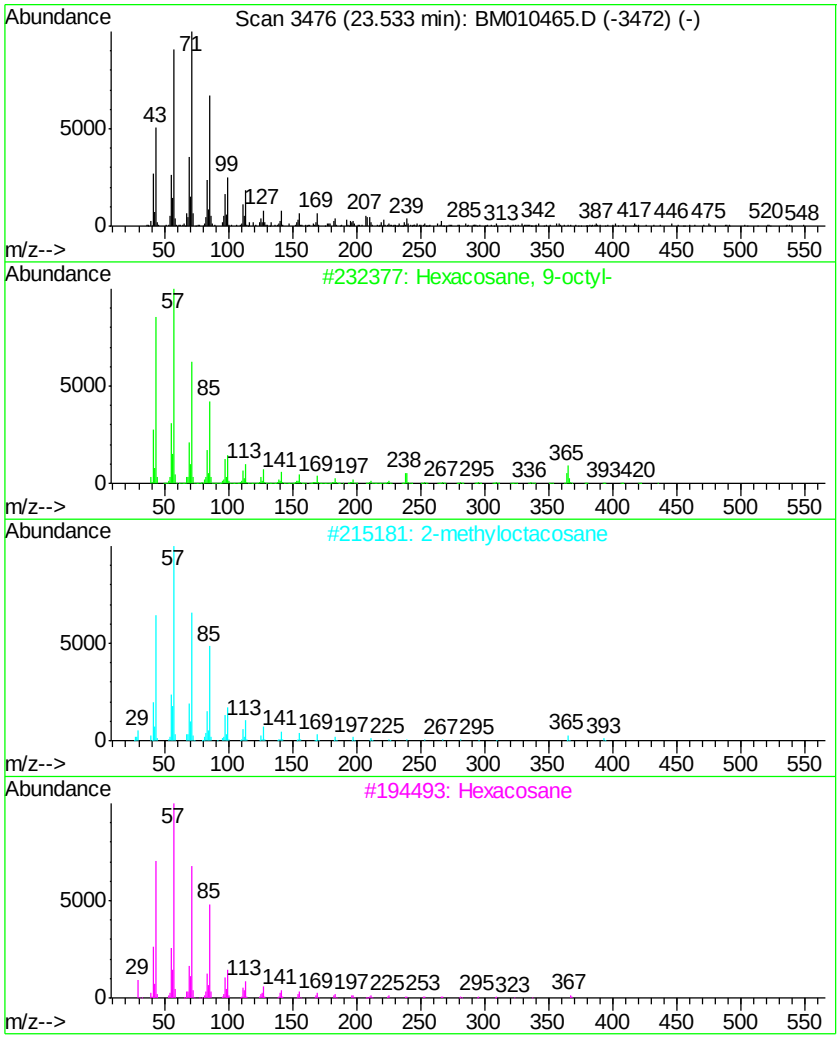
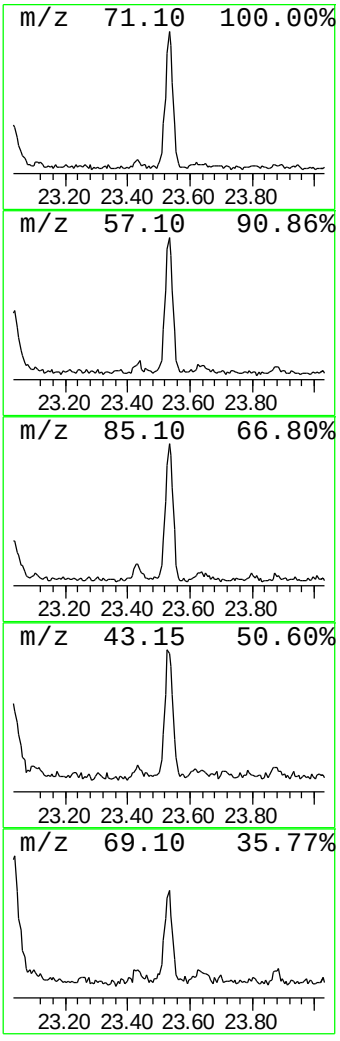
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.53	2.63 ng/ul	1457290	Perylene-d12	23.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane, 9-octyl-	479	C34H70	055429-83-9	83
2	2-methyloctacosane	408	C29H60	1000376-72-8	83
3	Hexacosane	366	C26H54	000630-01-3	83
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
5	Octacosane	394	C28H58	000630-02-4	83





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

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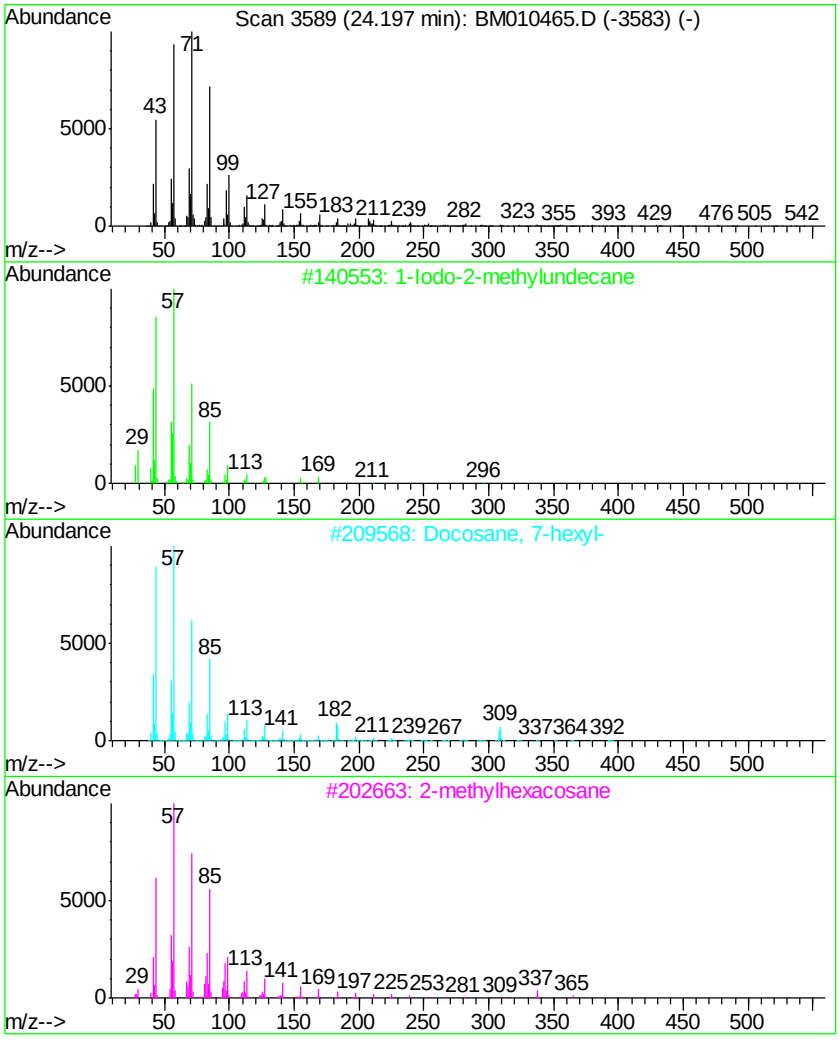
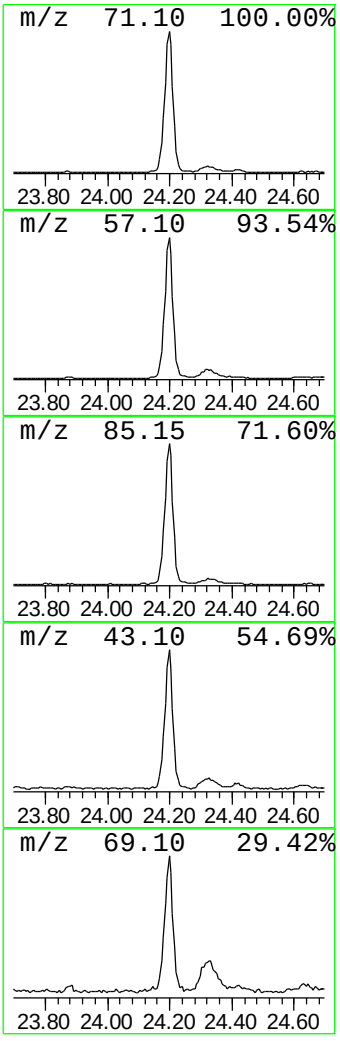
Peak Number 10 1-Iodo-2-methylundecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.20	12.69 ng/ul	7036340	Perylene-d12	23.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
2	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
3	2-methylhexacosane	380	C27H56	1000376-72-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010465.D
Acq On : 09 Jun 2017 22:03
Operator : SJ/MA
Sample : I3520-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F5A42

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.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
unknown-01	12.45	13.4	ng/ul	3798240	2	10.71	5676500	20.0
Tridecanoic acid	18.14	7.1	ng/ul	3893360	4	17.29	10950200	20.0
Octadecanoic acid	19.40	2.9	ng/ul	2005540	5	21.45	13971400	20.0
5-Bromo-4-oxo-4,5...	20.32	4.1	ng/ul	2895260	5	21.45	13971400	20.0
(DEL) Alkane: Cyc...	21.12	5.2	ng/ul	3657450	5	21.45	13971400	20.0
Ergosterol	22.01	4.0	ng/ul	2811030	5	21.45	13971400	20.0
(DEL) Alkane: Str...	22.96	10.1	ng/ul	5602210	6	23.80	11090400	20.0
(DEL) Alkane: Cyc...	23.03	2.6	ng/ul	1447760	6	23.80	11090400	20.0
(DEL) Alkane: Str...	23.53	2.6	ng/ul	1457290	6	23.80	11090400	20.0
1-Iodo-2-methylun...	24.20	12.7	ng/ul	7036340	6	23.80	11090400	20.0