LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023046.D
Acq On : 08 Oct 2019 15:35
Operator : JU
Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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	59	rVB	63048	92976	1.45%	0.151%
2	3.987	166	170	175	rVB	10587	14426	0.23%	0.024%
3	4.210	204	208	212	rVB3	7562	10306	0.16%	0.017%
4	6.775	641	644	652	rBV3	5819	11144	0.17%	0.018%
5	6.946	666	673	685	rBV	1012047	1644756	25.69%	2.680%
6	7.110	694	701	718	rBV	776135	1243348	19.42%	2.026%
7	7.310	728	735	748	rBV	1077073	1699811	26.55%	2.770%
8	7.775	807	814	822	rBV	681346	1044410	16.31%	1.702%
9	7.845	822	826	835	rVB	15590	26526	0.41%	0.043%
10	8.481	927	934	948	rBV	1216176	1984386	30.99%	3.233%
11	8.928	1002	1010	1023	rBV	965139	1555101	24.29%	2.534%
12	9.375	1080	1086	1091	rBV	7350	11578	0.18%	0.019%
13	9.651	1125	1133	1141	rBV	764830	1279066	19.98%	2.084%
14	9.887	1167	1173	1181	rBV	37526	68518	1.07%	0.112%
15	10.187	1217	1224	1236	rBV	1265888	2074541	32.40%	3.380%
16	10.563	1280	1288	1297	rBV	909023	1493740	23.33%	2.434%
17	10.698	1303	1311	1331	rBV	1155692	1999689	31.23%	3.258%
18	11.086	1372	1377	1382	rBV2	5249	12090	0.19%	0.020%
19	11.357	1418	1423	1428	rVB2	8378	12737	0.20%	0.021%
20	12.157	1552	1559	1564	rBV2	17875	27592	0.43%	0.045%
21	12.692	1644	1650	1660	rBV	37386	59733	0.93%	0.097%
22	13.028	1702	1707	1715	rVB6	5042	7744	0.12%	0.013%
23	13.633	1805	1810	1816	rBV2	12172	17909	0.28%	0.029%
24	13.822	1836	1842	1847	rBV	2022057	2738522	42.77%	4.462%
25	13.869	1847	1850	1859	rVB	272593	352106	5.50%	0.574%
26	14.104	1880	1890	1899	rBV	2566338	3590424	56.07%	5.850%
27	14.410	1936	1942	1951	rVV	1337047	1935474	30.23%	3.154%
28	14.604	1969	1975	1992	rBV	925644	1328427	20.75%	2.164%
29	14.839	2009	2015	2025	rBV	249824	353398	5.52%	0.576%
30	15.221	2076	2080	2084	rBV3	5150	7995	0.12%	0.013%
31	15.274	2084	2089	2092	rVB4	5791	9336	0.15%	0.015%
32	15.404	2105	2111	2118	rBV	3027628	4280280	66.85%	6.974%
33	15.521	2124	2131	2143	rBV	858986	1135393	17.73%	1.850%
34	15.645	2147	2152	2161	rVB	30753	46821	0.73%	0.076%

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ClientSampleId : DBAF0

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	16.133	2232	2235	2238	rBV3	7412	7823	0.12%	0.013%
36	16.186	2241	2244	2248	rVB3	10623	14138	0.22%	0.023%
37	16.557	2302	2307	2312	rBV	45442	59327	0.93%	0.097%
38	16.921	2362	2369	2376	rBV6	10247	22517	0.35%	0.037%
39	17.151	2402	2408	2414	rVV2	1591841	2200174	34.36%	3.585%
40	17.251	2418	2425	2434	rVV	3217088	4402937	68.76%	7.174%
41	17.327	2435	2438	2444	rVB4	8033	11787	0.18%	0.019%
42	17.539	2469	2474	2479	rBV6	12792	22511	0.35%	0.037%
43	17.657	2491	2494	2498	rVB3	7238	7482	0.12%	0.012%
44	17.827	2520	2523	2529	rBV7	4186	6608	0.10%	0.011%
45	17.921	2535	2539	2545	rBV4	16340	28702	0.45%	0.047%
46	17.986	2545	2550	2555	rBV3	12244	17968	0.28%	0.029%
47	18.051	2555	2561	2570	rBV	293710	412292	6.44%	0.672%
48	18.351	2609	2612	2614	rBV4	7231	10010	0.16%	0.016%
49	18.374	2614	2616	2621	rVB3	9333	14103	0.22%	0.023%
50	18.480	2630	2634	2639	rBV	24515	29213	0.46%	0.048%
51	18.757	2679	2681	2686	rBV5	4223	6785	0.11%	0.011%
52	18.804	2686	2689	2694	rBV6	7847	10547	0.16%	0.017%
53	18.909	2705	2707	2710	rBV4	5854	7503	0.12%	0.012%
54	18.945	2710	2713	2716	rVV4	8535	13233	0.21%	0.022%
55	18.986	2718	2720	2725	rVB3	8669	9390	0.15%	0.015%
56	19.109	2737	2741	2744	rBV6	6334	8752	0.14%	0.014%
57	19.180	2748	2753	2756	rVV	36489	55239	0.86%	0.090%
58	19.209	2756	2758	2767	rVB5	21420	33909	0.53%	0.055%
59	19.333	2774	2779	2791	rBV	118779	179478	2.80%	0.292%
60	19.433	2792	2796	2801	rVB	33283	40690	0.64%	0.066%
61	19.545	2809	2815	2822	rBV	4065510	5432744	84.85%	8.852%
62	19.604	2822	2825	2831	rVB5	25434	40851	0.64%	0.067%
63	19.886	2869	2873	2876	rBV	333185	362540	5.66%	0.591%
64	19.927	2876	2880	2884	rVB	606586	667268	10.42%	1.087%
65	20.098	2907	2909	2914	rVB5	14678	15978	0.25%	0.026%
66	20.862	3035	3039	3042	rBV	280833	295603	4.62%	0.482%
67	20.898	3042	3045	3049	rVB	458599	490340	7.66%	0.799%
68	21.056	3067	3072	3079	rBV2	166465	269176	4.20%	0.439%
69	21.333	3114	3119	3125	rBV	2065334	2663343	41.59%	4.339%
70	21.498	3144	3147	3149	rBV	71548	71136	1.11%	0.116%
71	21.733	3184	3187	3190	rBV	186447	223223	3.49%	0.364%

LSC Area Percent Report

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Instrument : BNA_M
ClientSampleId : DBAF0

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

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Peak separation: 5

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

72	21.768	3190	3193	3199	rVB	241548	281228	4.39%	0.458%
73	21.933	3218	3221	3227	rBV	132243	160041	2.50%	0.261%
74	22.397	3297	3300	3306	rVB	198379	232469	3.63%	0.379%
75	22.527	3320	3322	3328	rVB	114646	131286	2.05%	0.214%
76	22.709	3349	3353	3359	rVB	197688	273734	4.28%	0.446%
77	22.909	3383	3387	3393	rBV	239606	328608	5.13%	0.535%
78	23.450	3471	3479	3494	rVB	3212756	6403039	100.00%	10.433%
79	23.592	3496	3503	3511	rVB	1507117	2839081	44.34%	4.626%
80	24.139	3592	3596	3603	rVB	222006	390161	6.09%	0.636%

Sum of corrected areas: 61375270

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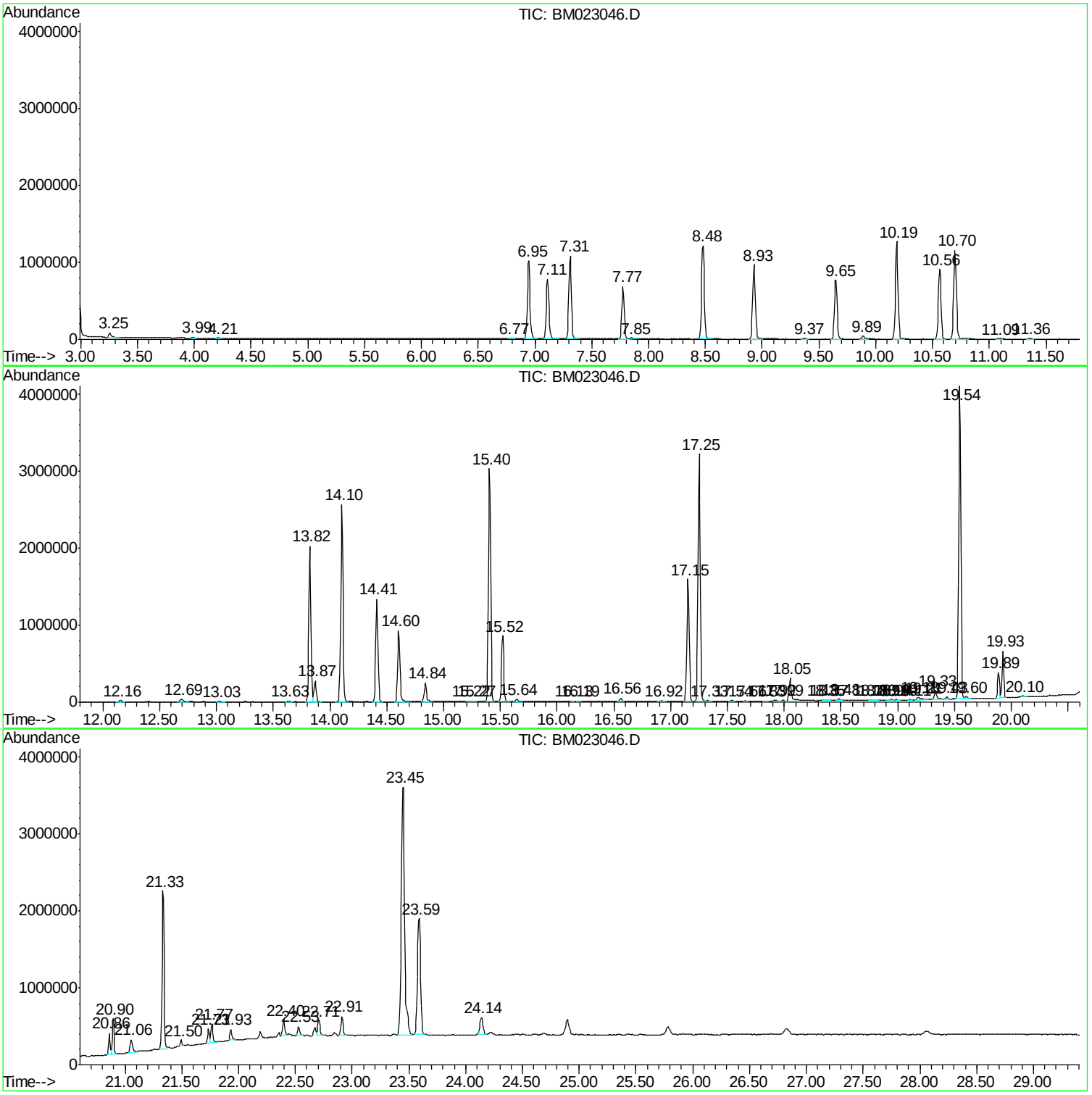
Instrument :
BNA_M
ClientSampleId :
DBAF0

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\
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Acq On : 08 Oct 2019 15:35
Operator : JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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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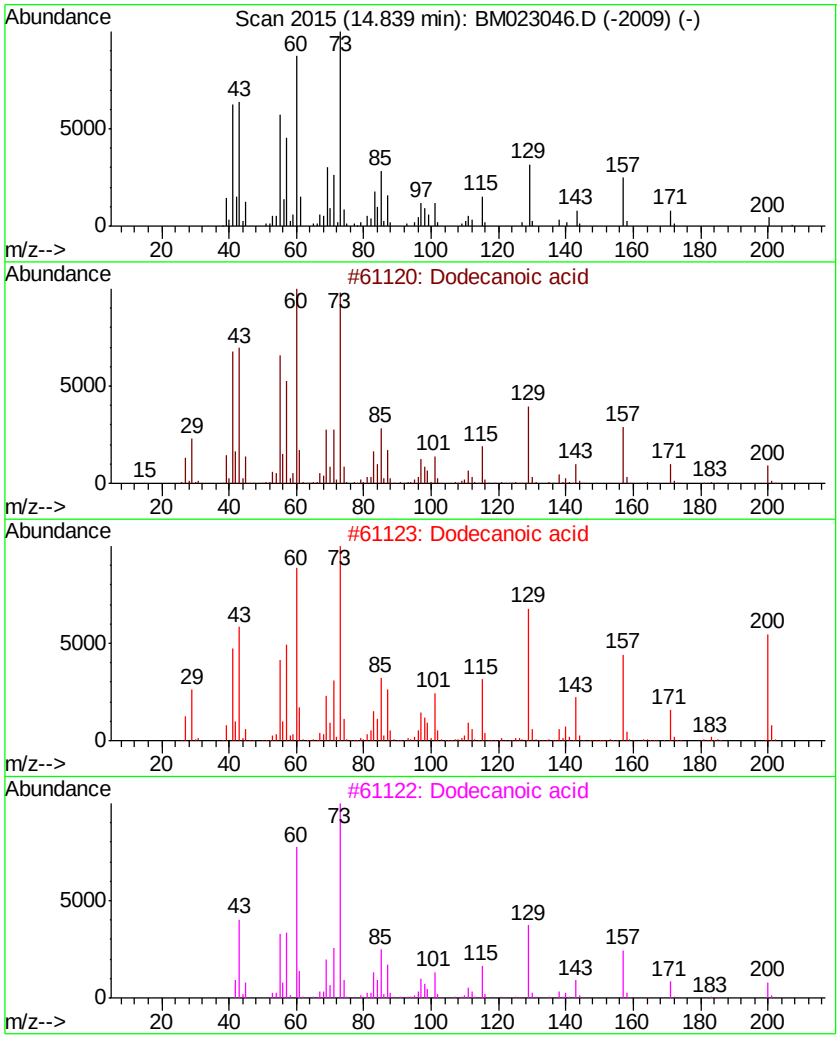
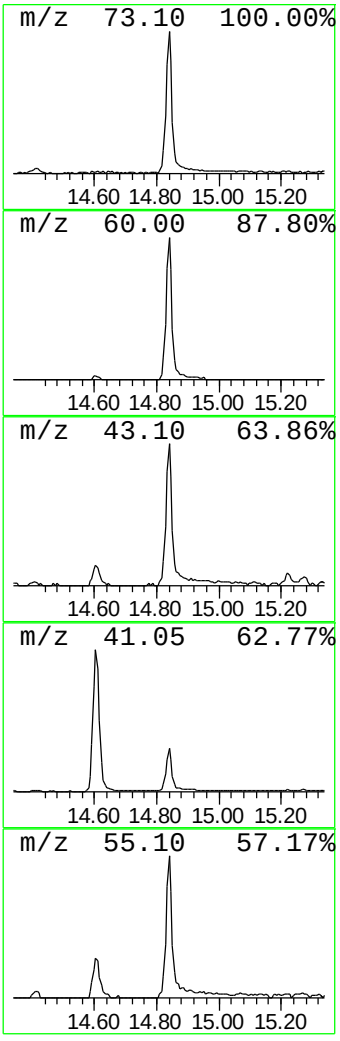
Peak Number 1 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.65 ng/ul	353398	Acenaphthene-d10	14.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	94
3	Dodecanoic acid	200	C12H24O2	000143-07-7	91
4	Dodecanoic acid	200	C12H24O2	000143-07-7	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Library Search Compound Report

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Data File : BM023046.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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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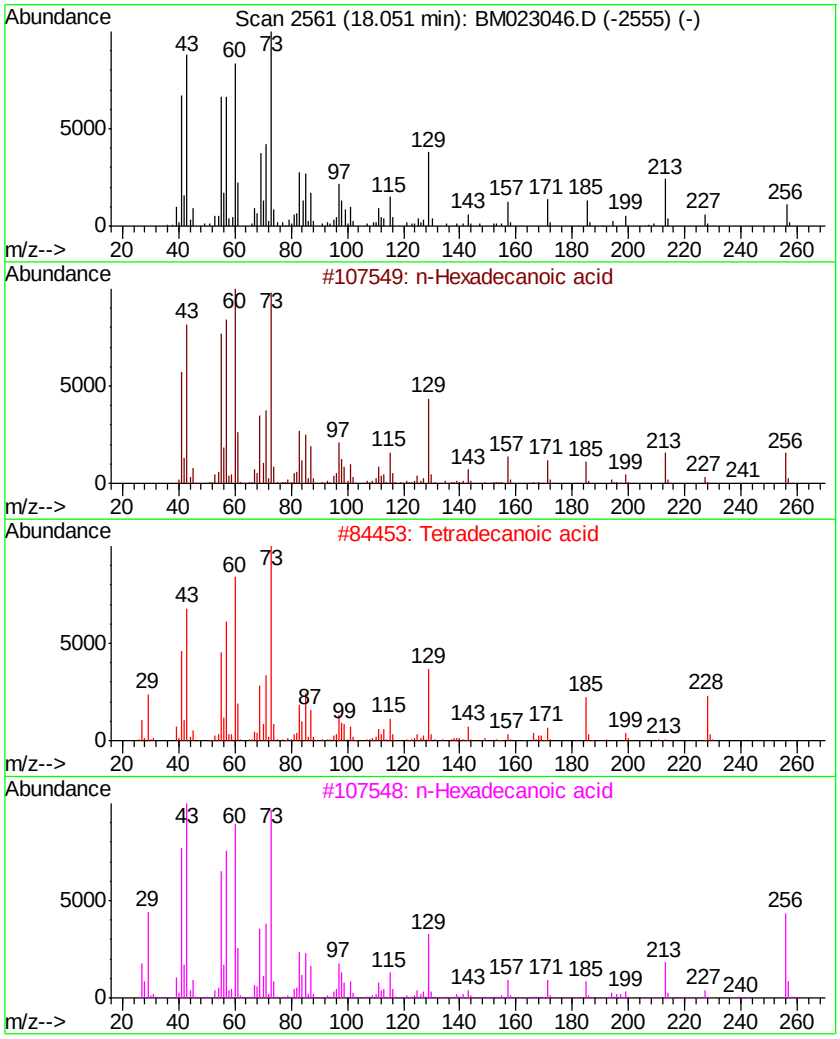
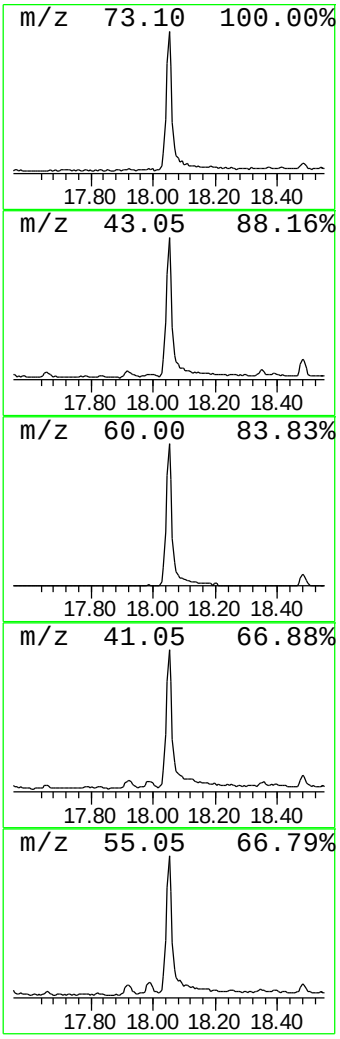
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	3.75 ng/ul	412292	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Library Search Compound Report

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ALS Vial : 14 Sample Multiplier: 1

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

TIC Library : C:\DATABASE\NIST11.L
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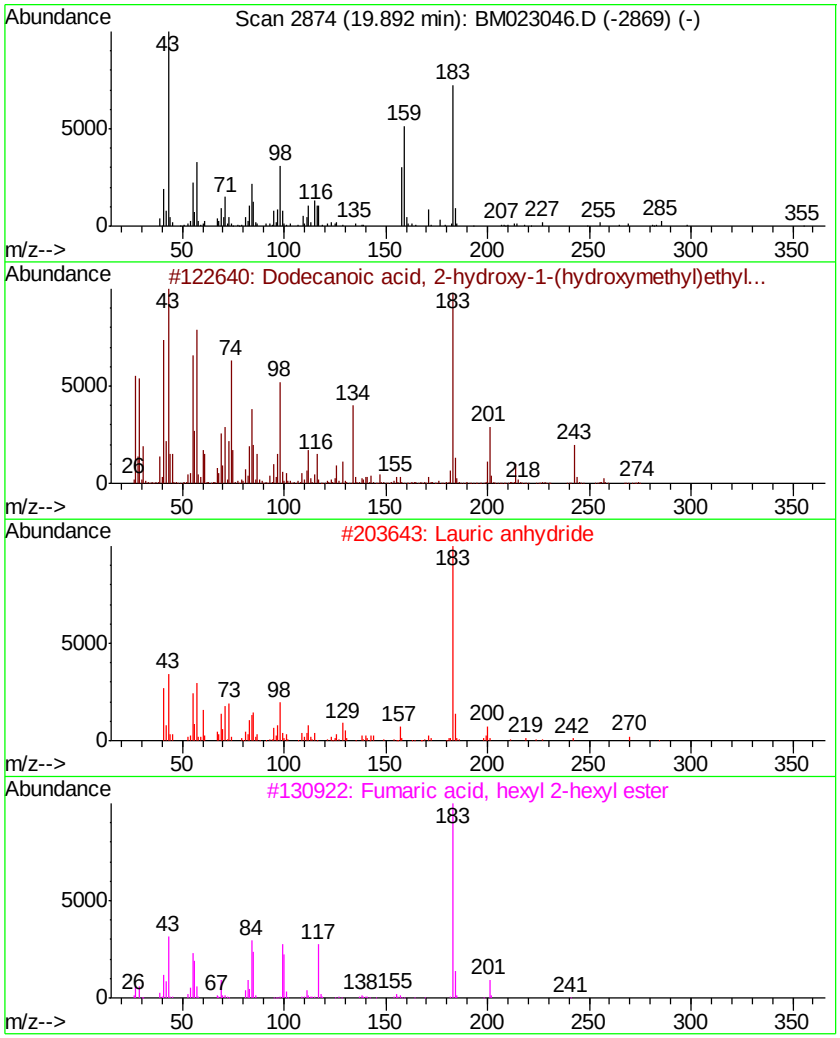
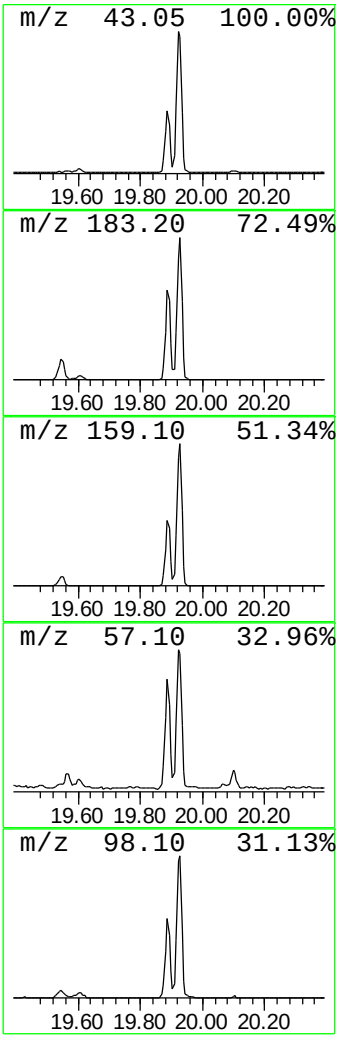
****

Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	2.72 ng/ul	362540	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	47
2	Lauric anhydride	382	C24H46O3	000645-66-9	38
3	Fumaric acid, hexyl 2-hexyl ester	284	C16H28O4	1000348-74-5	27
4	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	25
5	Fumaric acid, di(3-hexyl) ester	284	C16H28O4	1000348-61-9	22





Library Search Compound Report

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Quant Title : SVOA CALIBRATION

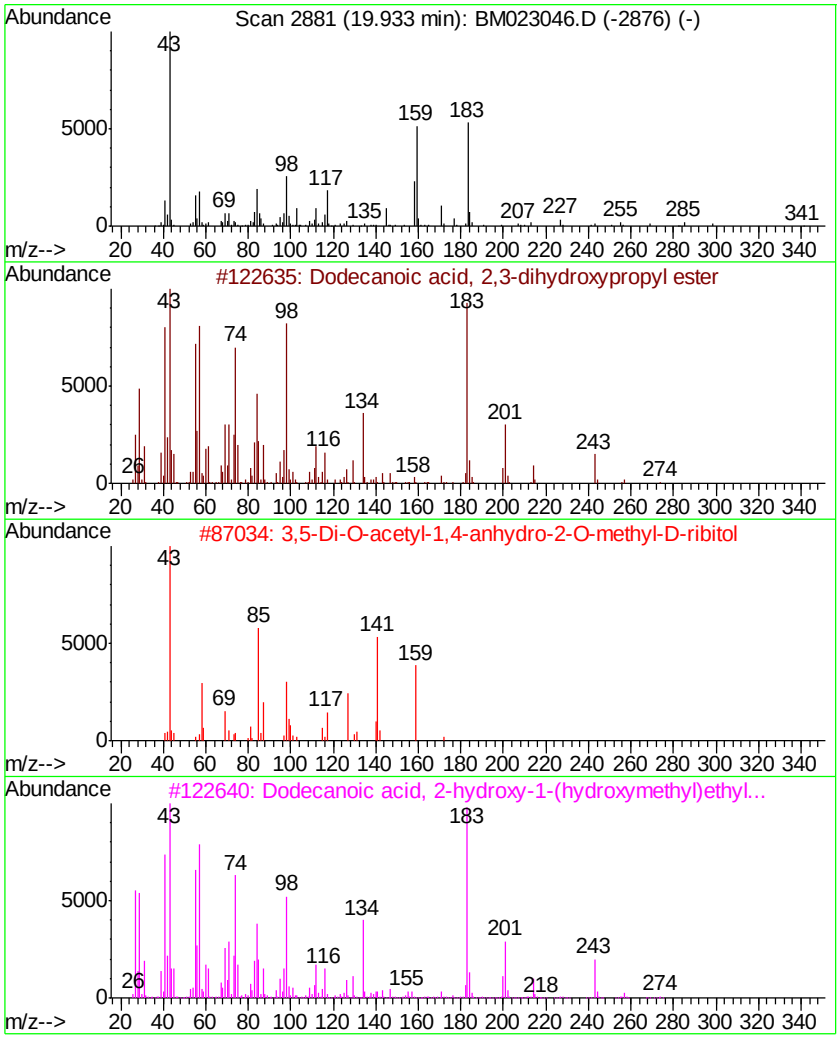
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

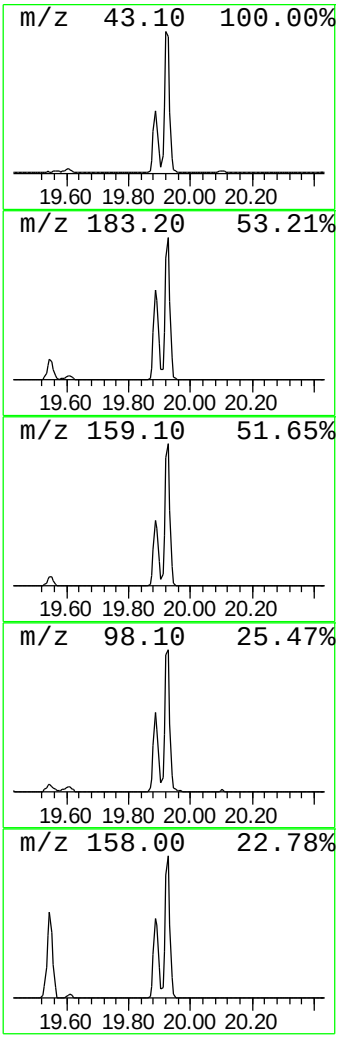
****

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.93	5.01 ng/ul	667268	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	22
2	3,5-Di-O-acetyl-1,4-anhydro-2-O-...	232	C10H16O6	1000357-23-2	17
3	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	16
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10
5	5-Isoxazolidinemethanol, 2-acety...	201	C9H15NO4	064018-47-9	9





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Instrument : BNA_M
ClientSampleId : DBAF0

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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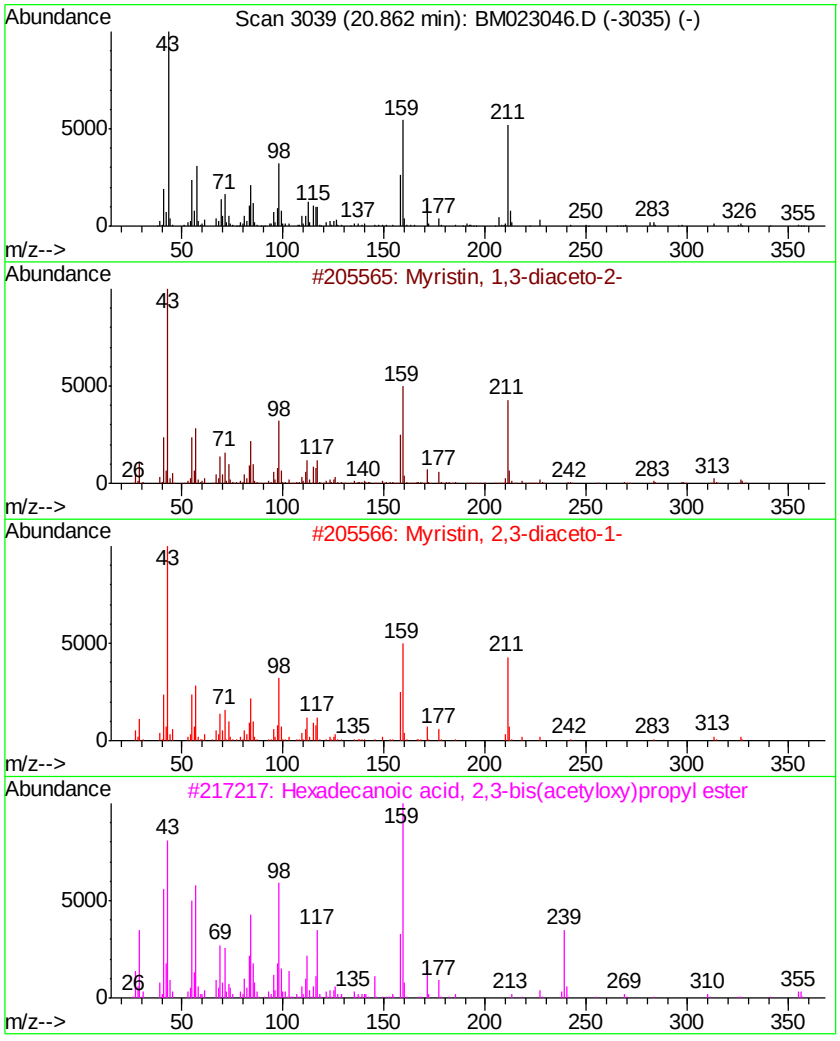
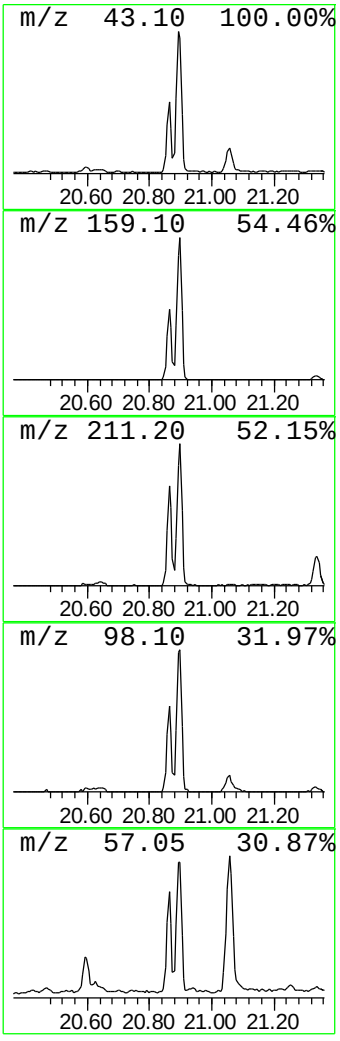
Peak Number 5 Myristin, 1,3-diaceto-2- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.22 ng/ul	295603	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
2	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	90
3	Hexadecanoic acid, 2,3-bis(acetv...	414	C23H42O6	055268-70-7	52
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	30
5	Diethylmalonic acid, hexyl 4-tri...	402	C21H29F3O4	1000368-40-4	14





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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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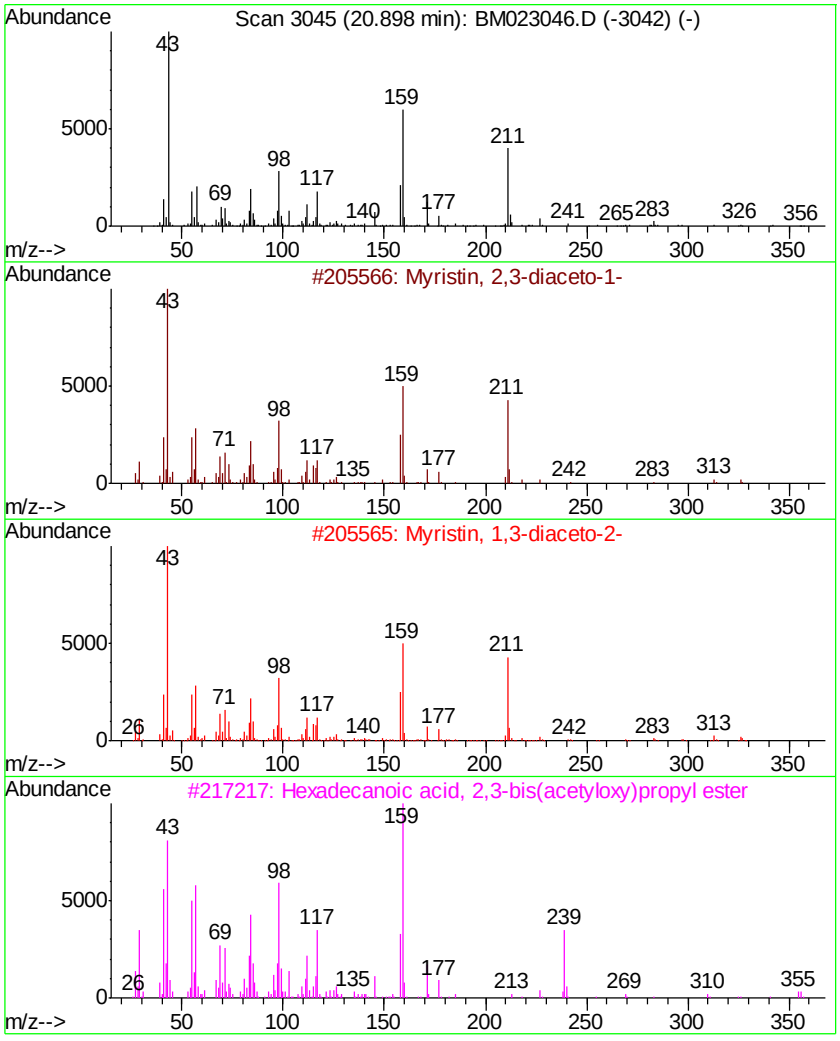
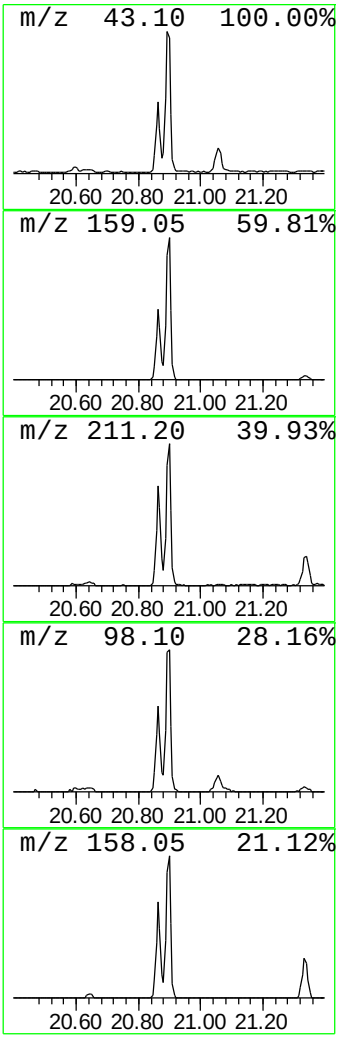
Peak Number 6 Myristin, 2,3-diaceto-1- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	3.68 ng/ul	490340	Chrysene-d12	21.33

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	50
3	Hexadecanoic acid, 2,3-bis(acetv...	414	C23H42O6	055268-70-7	49
4	2,5-Difluorobenzoic acid, tetrad...	354	C21H32F2O2	1000338-81-3	14
5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM100819\
Data File : BM023046.D
Acq On : 08 Oct 2019 15:35
Operator : JU
Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

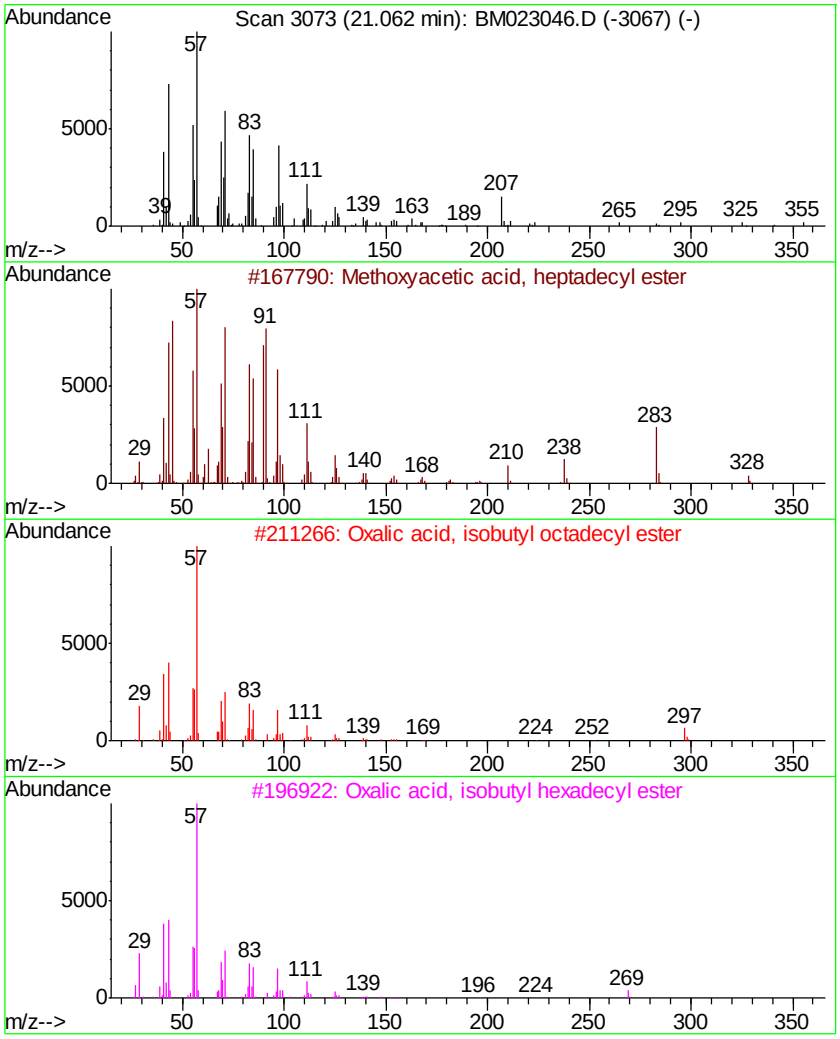
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

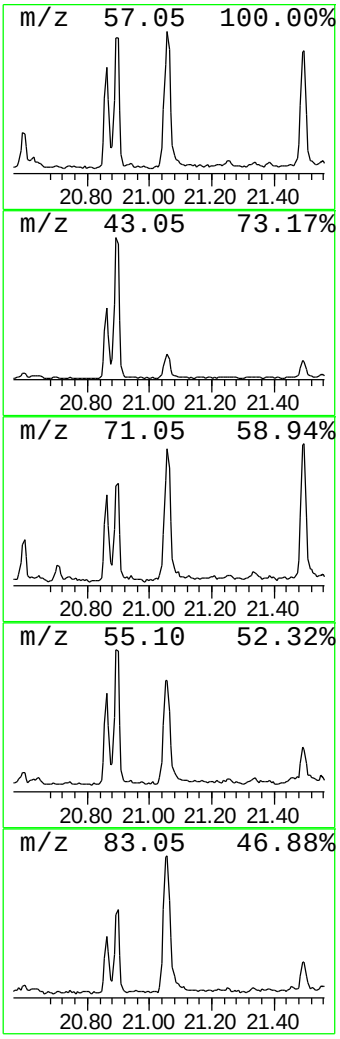
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Methoxyacetic acid, heptade... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	2.02 ng/ul	269176	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	91
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81





Library Search Compound Report

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Data File : BM023046.D
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Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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

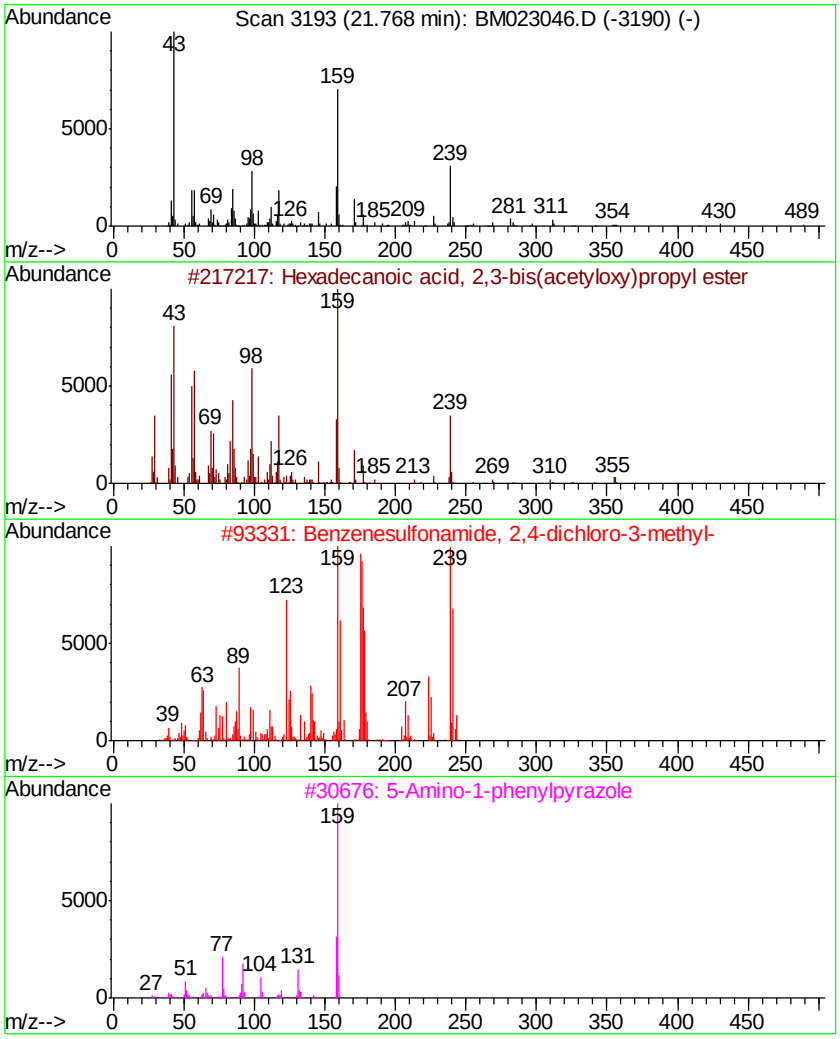
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

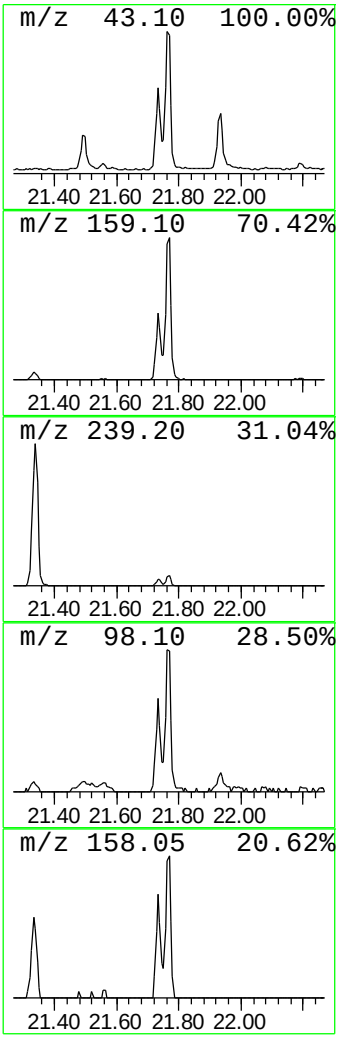
****

Peak Number 8 Hexadecanoic acid, 2,3-bis(... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	2.11 ng/ul	281228	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2,3-bis(acetv...	414	C23H42O6	055268-70-7	91
2	Benzenesulfonamide, 2,4-dichloro...	239	C7H7Cl2NO2S	1000277-29-3	38
3	5-Amino-1-phenylpyrazole	159	C9H9N3	000826-85-7	27
4	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	25
5	4-Trifluoromethylbenzyl bromide	238	C8H6BrF3	000402-49-3	14





Library Search Compound Report

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Data File : BM023046.D
Acq On : 08 Oct 2019 15:35
Operator : JU
Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

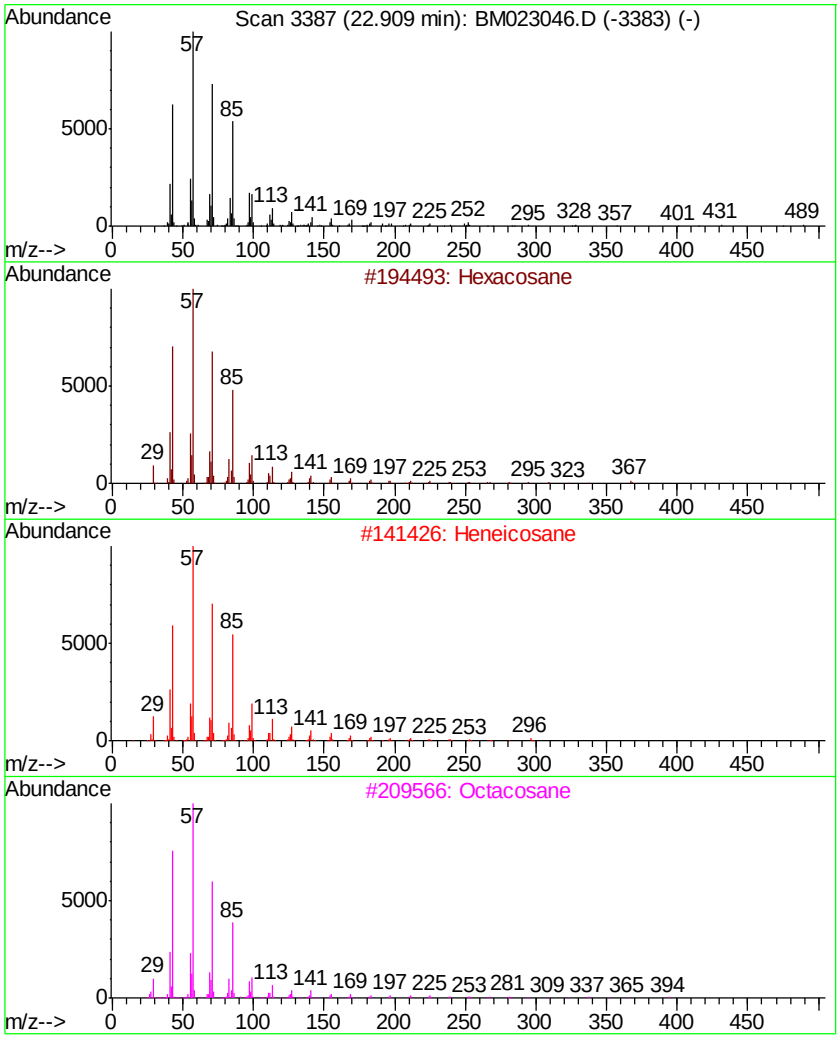
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

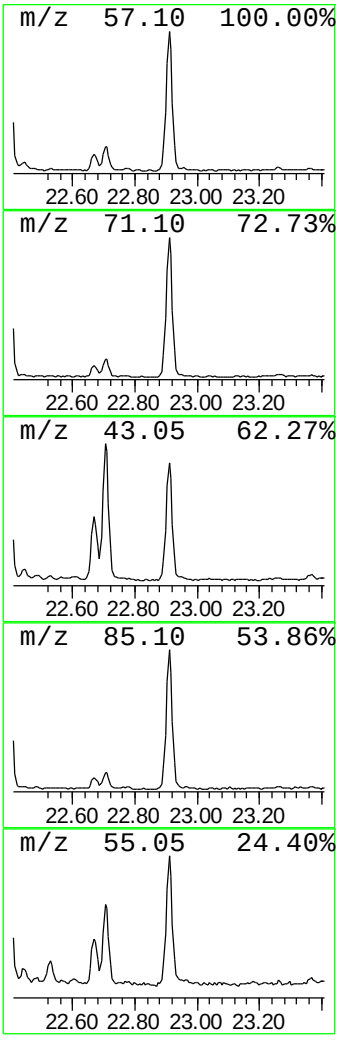
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.91	2.31 ng/ul	328608	Perylene-d12	23.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





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Operator : JU
Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

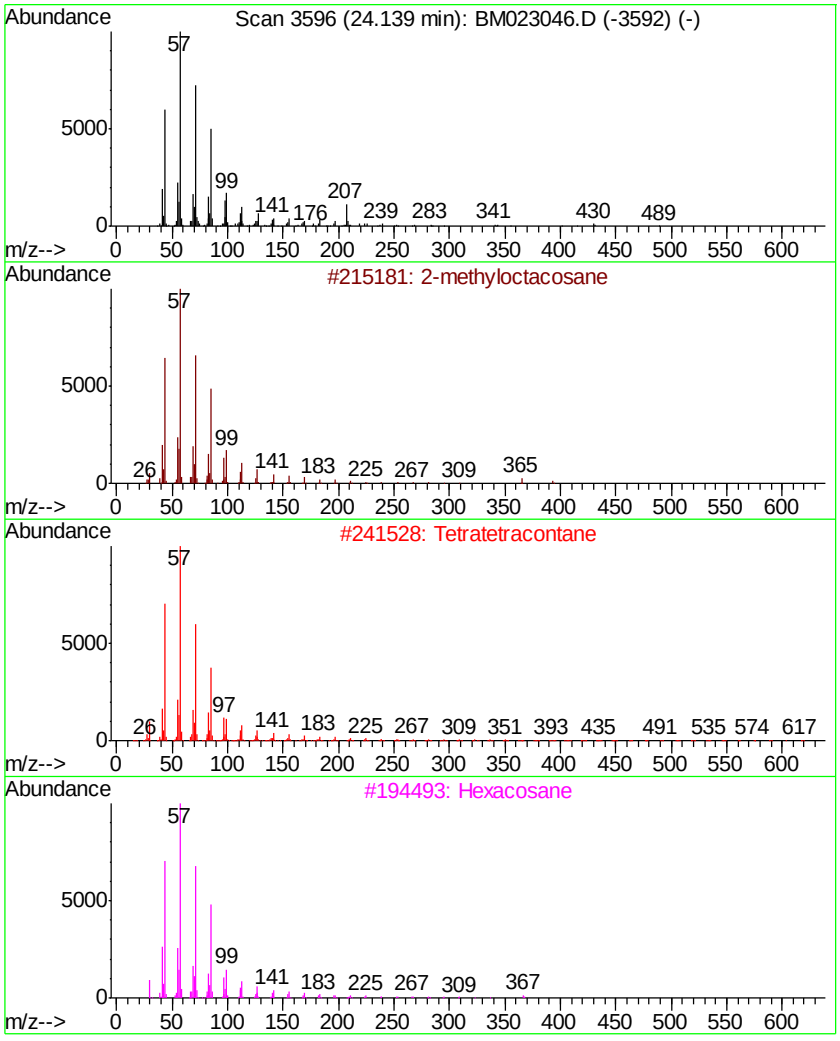
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM092719MA.M
Quant Title : SVOA CALIBRATION

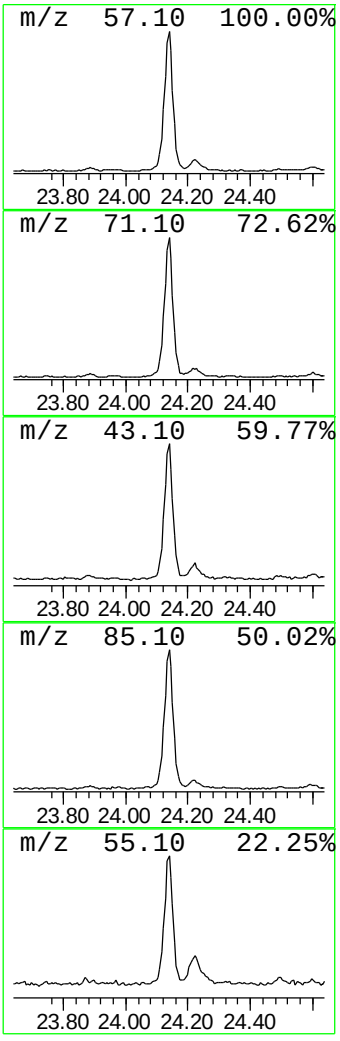
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	2.75 ng/ul	390161	Perylene-d12	23.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane	394	C28H58	000630-02-4	83
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

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Data File : BM023046.D
Acq On : 08 Oct 2019 15:35
Operator : JU
Sample : K5056-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DBAF0

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	3.6	ng/ul	353398	3	14.41	1935470	20.0
n-Hexadecanoic acid	18.05	3.8	ng/ul	412292	4	17.15	2200170	20.0
unknown-01	19.89	2.7	ng/ul	362540	5	21.33	2663340	20.0
unknown-02	19.93	5.0	ng/ul	667268	5	21.33	2663340	20.0
Myristin, 1,3-dia...	20.86	2.2	ng/ul	295603	5	21.33	2663340	20.0
Myristin, 2,3-dia...	20.90	3.7	ng/ul	490340	5	21.33	2663340	20.0
Methoxyacetic aci...	21.06	2.0	ng/ul	269176	5	21.33	2663340	20.0
Hexadecanoic acid...	21.77	2.1	ng/ul	281228	5	21.33	2663340	20.0
(DEL) Alkane: Str...	22.91	2.3	ng/ul	328608	6	23.59	2839080	20.0
(DEL) Alkane: Str...	24.14	2.8	ng/ul	390161	6	23.59	2839080	20.0