LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM050218\
Data File : BM014924.D
Acq On : 02 May 2018 15:56
Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

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-BM041918.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	3.340	4	9	25	rVB	2728258	3818224	66.21%	4.195%
2	3.640	56	60	69	rVB	92668	131108	2.27%	0.144%
3	4.716	238	243	248	rVB	60469	89592	1.55%	0.098%
4	5.157	313	318	326	rBV	44993	73455	1.27%	0.081%
5	5.481	366	373	383	rBV	227415	363008	6.29%	0.399%
6	6.504	543	547	556	rBV	36300	62442	1.08%	0.069%
7	7.134	649	654	659	rVB	53247	83241	1.44%	0.091%
8	7.616	729	736	753	rBV	1500746	2623654	45.49%	2.883%
9	7.798	760	767	780	rBV	1199389	1890595	32.78%	2.077%
10	7.916	780	787	793	rVB3	38130	68187	1.18%	0.075%
11	8.010	796	803	810	rBV	1530251	2483588	43.06%	2.729%
12	8.069	810	813	821	rVB2	51985	93291	1.62%	0.102%
13	8.492	878	885	898	rBV	1527358	2510093	43.52%	2.758%
14	9.192	996	1004	1014	rBV	1655961	2775037	48.12%	3.049%
15	9.675	1078	1086	1094	rBV	1414223	2354698	40.83%	2.587%
16	10.034	1140	1147	1153	rBV	42714	66771	1.16%	0.073%
17	10.404	1200	1210	1219	rBV	1097265	1835667	31.83%	2.017%
18	10.939	1292	1301	1317	rBV	1630158	2850537	49.43%	3.132%
19	11.333	1360	1368	1382	rBV	1985482	3496456	60.63%	3.842%
20	11.463	1382	1390	1407	rBV	1471474	2594437	44.99%	2.851%
21	13.898	1797	1804	1810	rBV	56721	81832	1.42%	0.090%
22	14.492	1896	1905	1909	rBV	2653844	3814144	66.14%	4.191%
23	14.533	1909	1912	1918	rVB	674589	937266	16.25%	1.030%
24	14.798	1951	1957	1967	rBV	3187205	4713362	81.73%	5.179%
25	14.951	1978	1983	1991	rVB	199652	251534	4.36%	0.276%
26	15.039	1991	1998	2002	rBV5	35410	69574	1.21%	0.076%
27	15.098	2002	2008	2015	rVB2	2734581	4137193	71.74%	4.546%
28	15.257	2029	2035	2051	rBV	1047171	1595237	27.66%	1.753%
29	15.845	2131	2135	2138	rBV	49799	68306	1.18%	0.075%
30	15.886	2138	2142	2147	rVB	226006	287248	4.98%	0.316%
31	16.074	2168	2174	2181	rBV	3894057	5534745	95.97%	6.081%
32	16.174	2185	2191	2203	rBV	942608	1327785	23.02%	1.459%
33	16.286	2204	2210	2213	rBV	49451	106533	1.85%	0.117%
34	16.515	2244	2249	2255	rVB3	120450	171324	2.97%	0.188%

LSC Area Percent Report

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Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

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-BM041918.M
Title : SVOA CALIBRATION

35	16.739	2282	2287	2297	rBV	180002	280818	4.87%	0.309%
36	17.521	2416	2420	2425	rBV	101088	124063	2.15%	0.136%
37	17.810	2463	2469	2475	rBV2	2882427	4383574	76.01%	4.816%
38	17.857	2475	2477	2480	rVV	69687	77350	1.34%	0.085%
39	17.910	2480	2486	2497	rVB2	3899998	5614381	97.35%	6.169%
40	18.251	2540	2544	2549	rBV	65671	78603	1.36%	0.086%
41	18.639	2605	2610	2621	rBV	799017	1211317	21.00%	1.331%
42	19.745	2794	2798	2800	rBV3	56282	78424	1.36%	0.086%
43	19.786	2800	2805	2808	rVV3	72919	154049	2.67%	0.169%
44	19.821	2808	2811	2816	rVB	91390	116991	2.03%	0.129%
45	19.880	2817	2821	2829	rBV	388271	530997	9.21%	0.583%
46	20.151	2861	2867	2876	rBV	4328854	5767101	100.00%	6.336%
47	21.556	3102	3106	3121	rVB	1004119	1492016	25.87%	1.639%
48	21.903	3159	3165	3170	rBV	2993102	4222617	73.22%	4.639%
49	23.239	3389	3392	3398	rVB	359422	518347	8.99%	0.570%
50	23.544	3441	3444	3449	rVB	264862	356657	6.18%	0.392%
51	23.603	3449	3454	3470	rVB2	895880	1826703	31.67%	2.007%
52	24.221	3552	3559	3573	rVB	2615202	5444436	94.41%	5.982%
53	24.380	3579	3586	3599	rVB	1967756	4119440	71.43%	4.526%
54	24.915	3672	3677	3686	rVB	628881	1258706	21.83%	1.383%

Sum of corrected areas: 91016754

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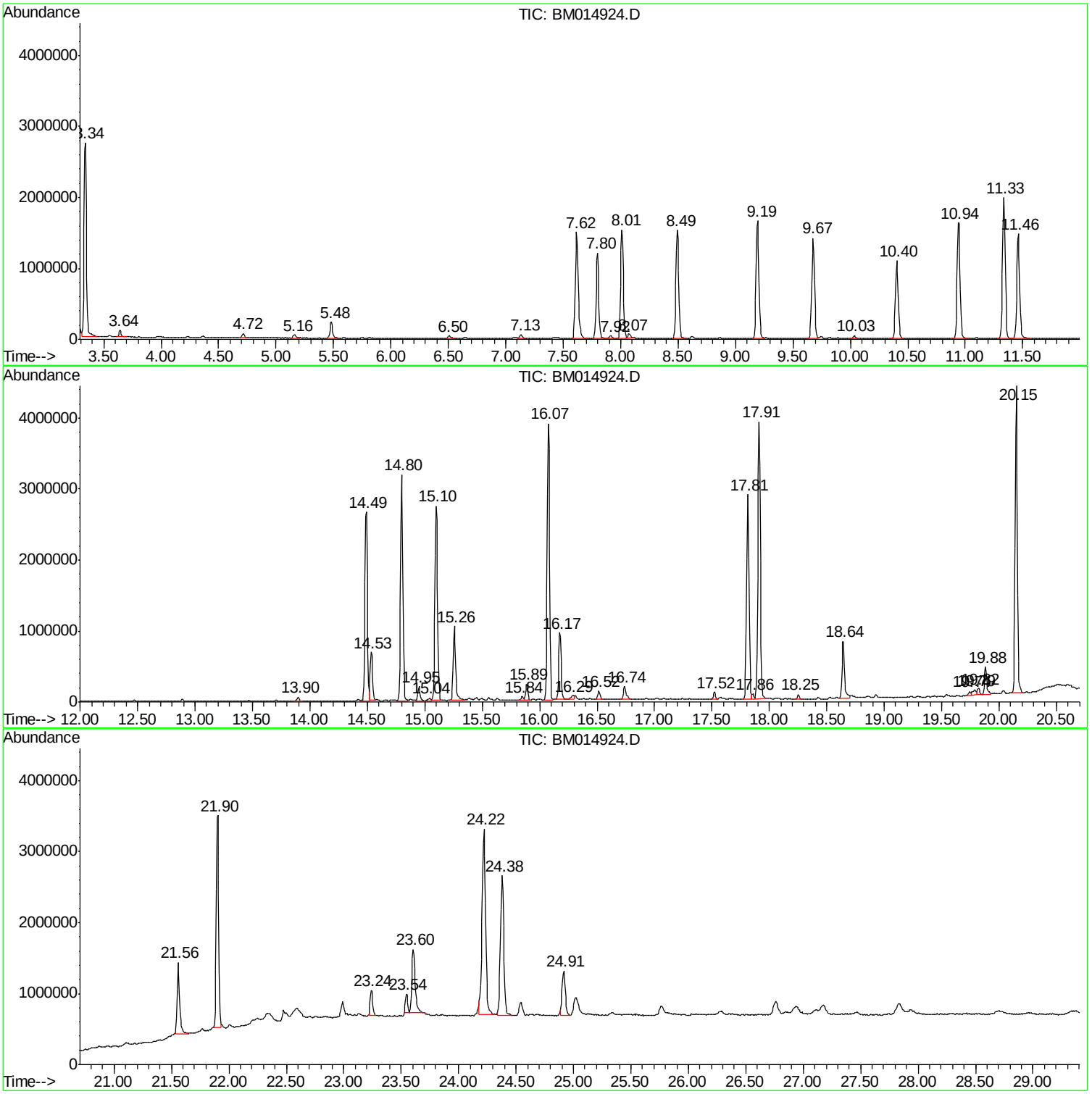
Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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



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Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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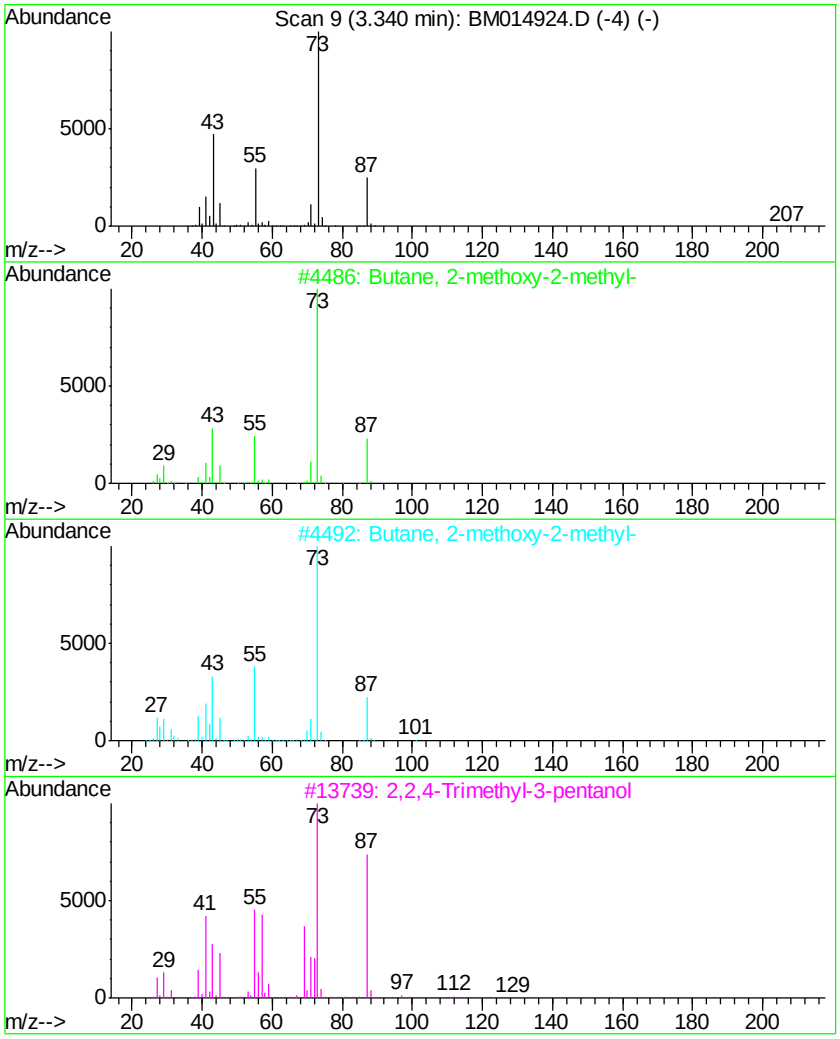
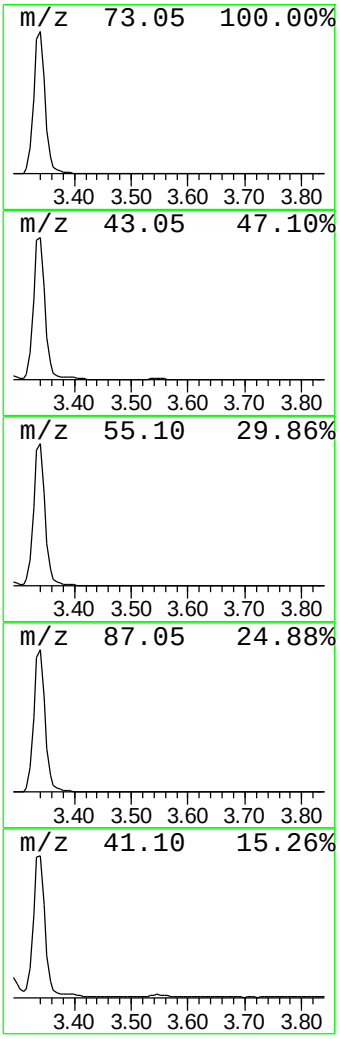
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.34	30.42 ng/ul	3818220	1,4-Dichlorobenzene-d4	8.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38





Library Search Compound Report

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Data File : BM014924.D
Acq On : 02 May 2018 15:56
Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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

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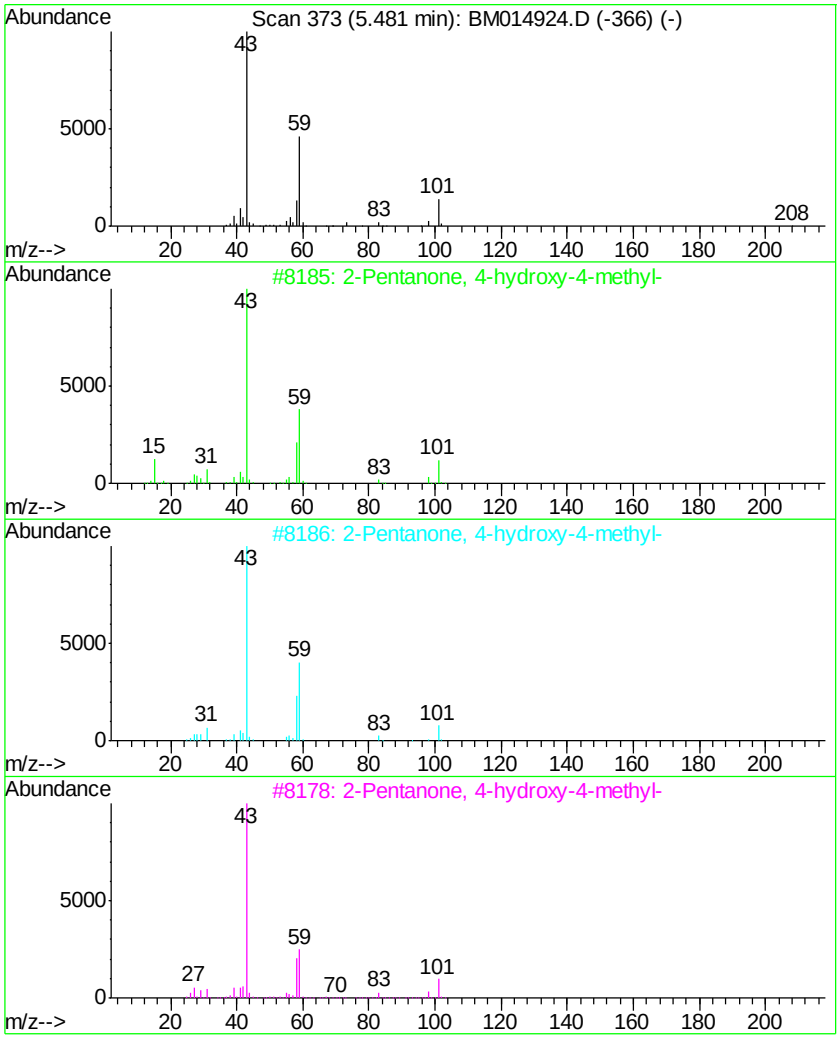
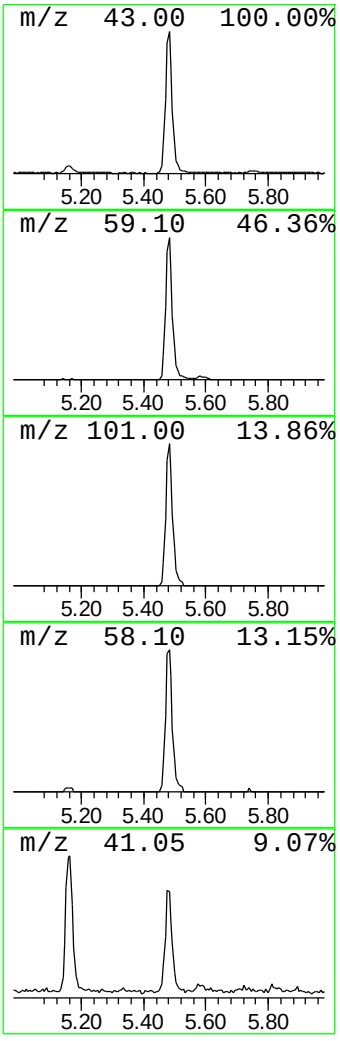
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.48	2.89 ng/ul	363008	1,4-Dichlorobenzene-d4	8.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	12





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Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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

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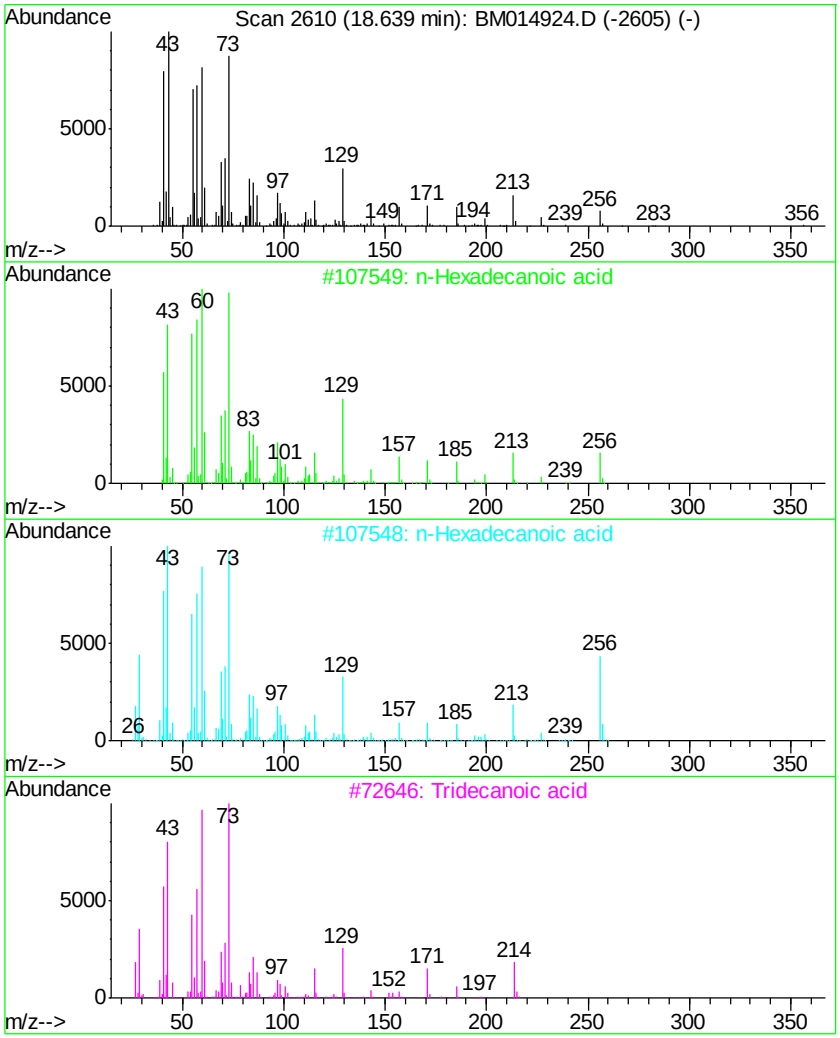
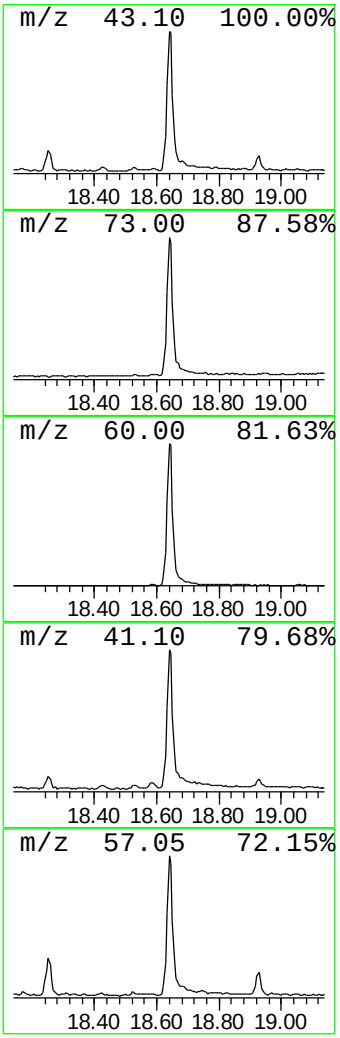
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.64	5.53 ng/ul	1211320	Phenanthrene-d10	17.81

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	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





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Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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

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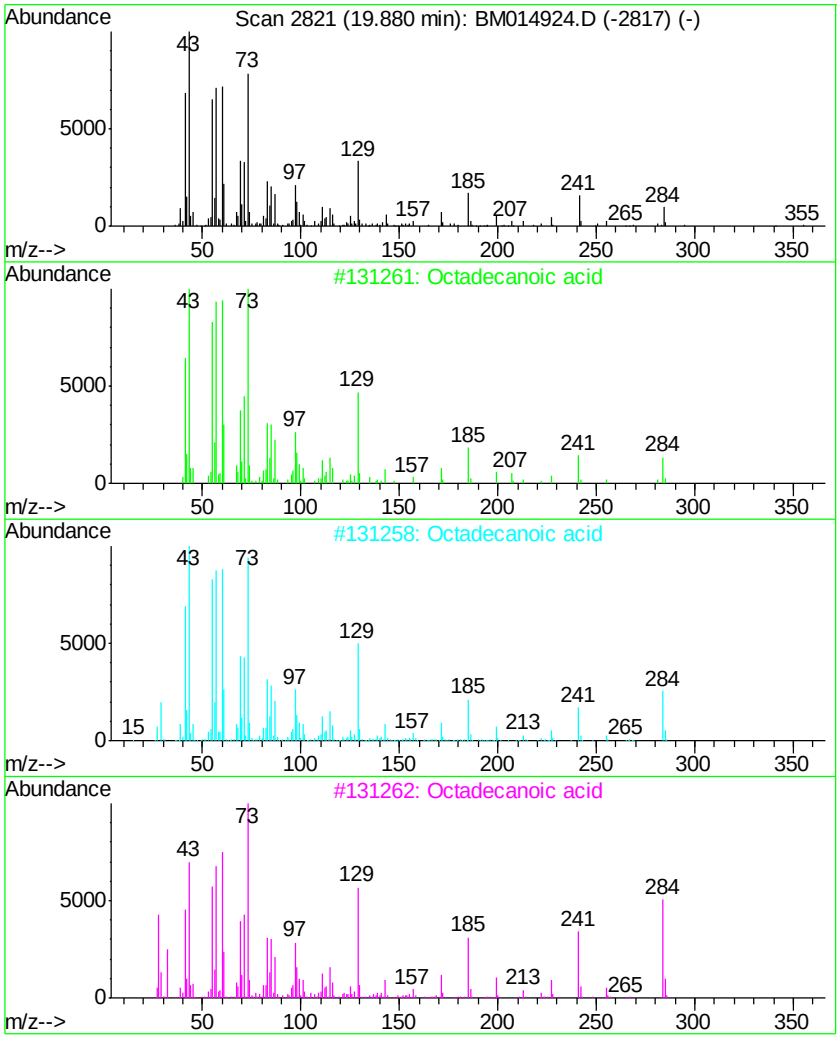
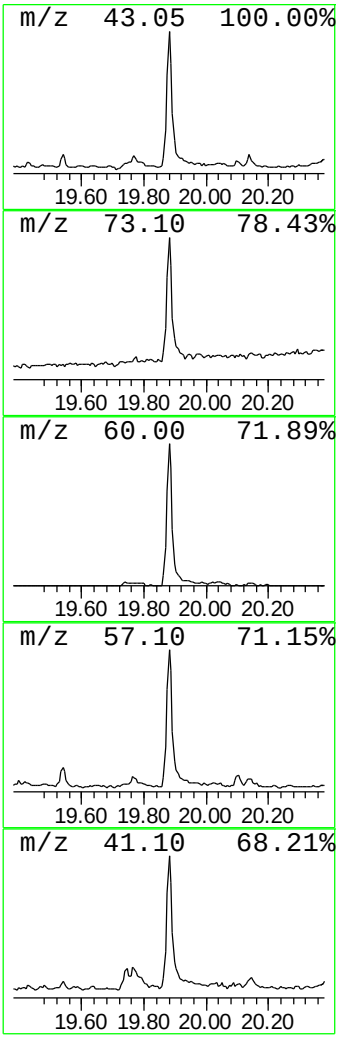
Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.88	2.52 ng/ul	530997	Chrysene-d12	21.90

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	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	86





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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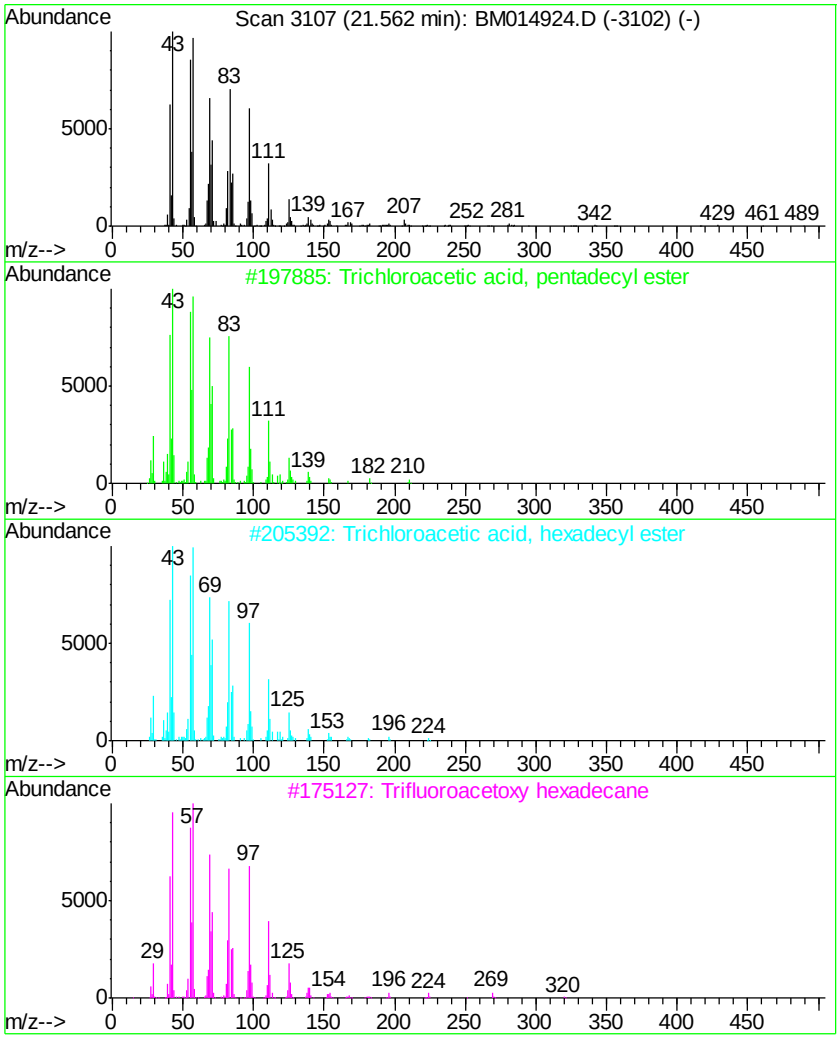
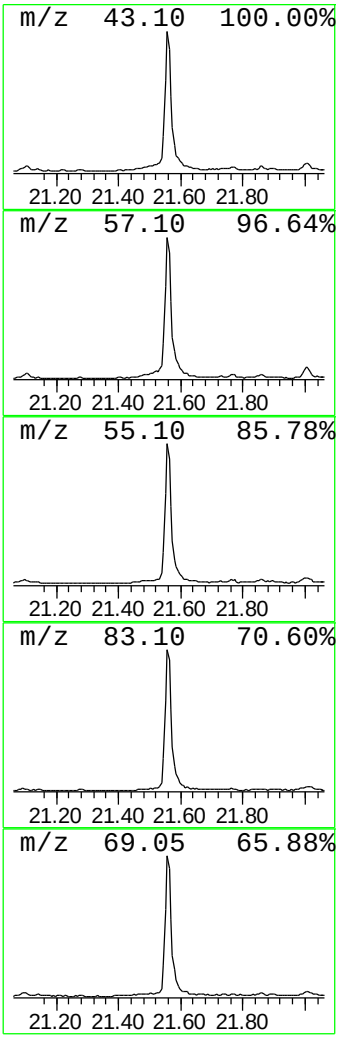
Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.56	7.07 ng/ul	1492020	Chrysene-d12	21.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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

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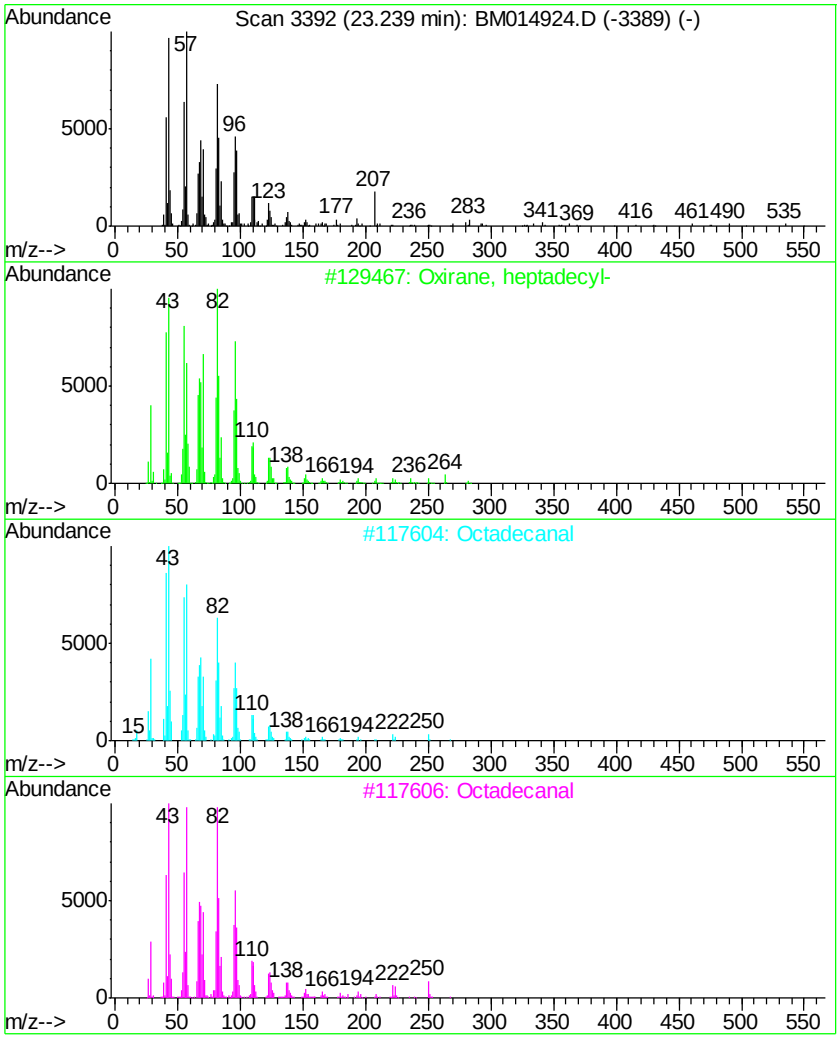
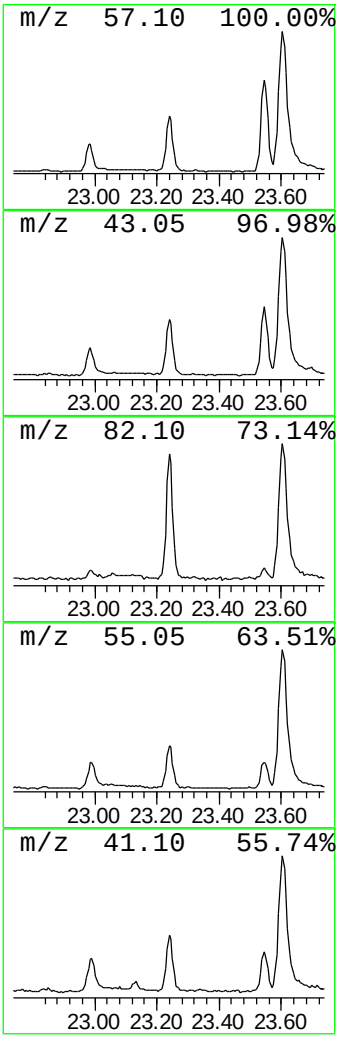
Peak Number 6 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.24	2.52 ng/ul	518347	Perylene-d12	24.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Octadecanal	268	C18H36O	000638-66-4	93
3	Octadecanal	268	C18H36O	000638-66-4	93
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	89
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87





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Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

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

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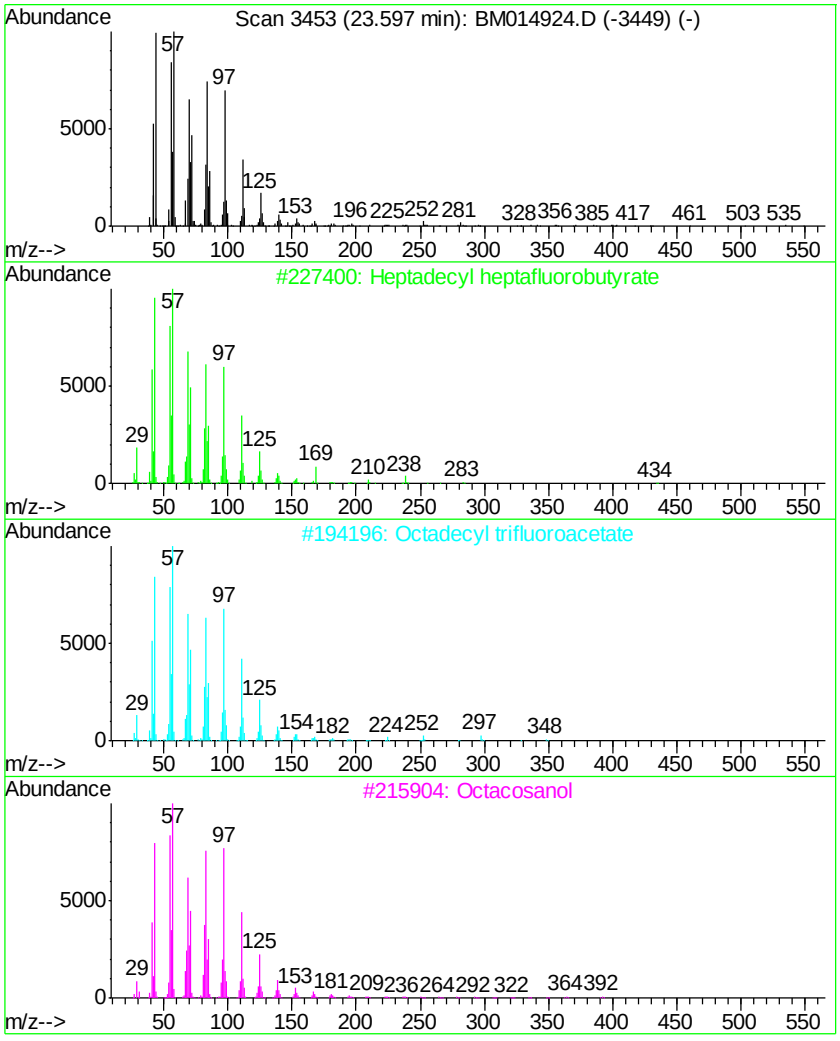
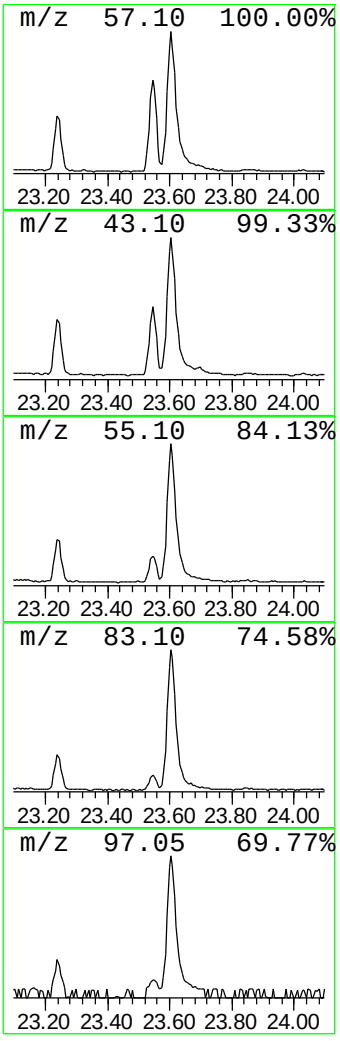
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.60	8.87 ng/ul	1826700	Perylene-d12	24.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Octacosanol	410	C28H58O	000557-61-9	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





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Data File : BM014924.D
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Misc :
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Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.M
Quant Title : SVOA CALIBRATION

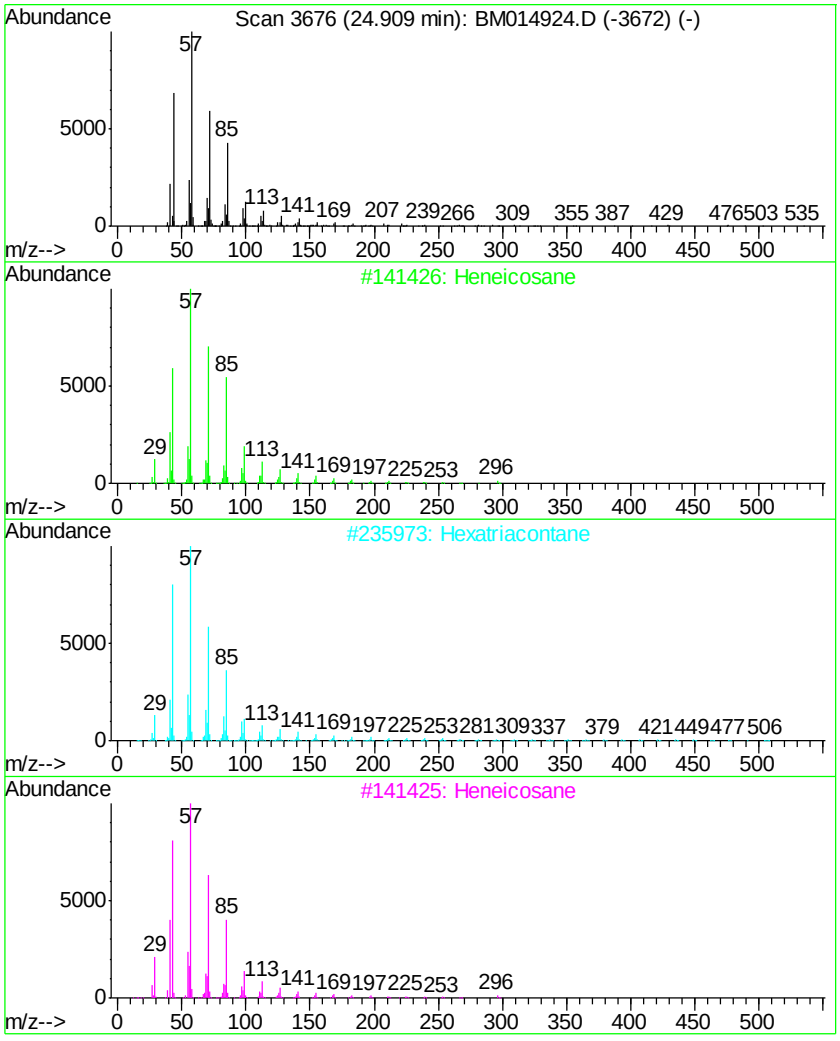
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

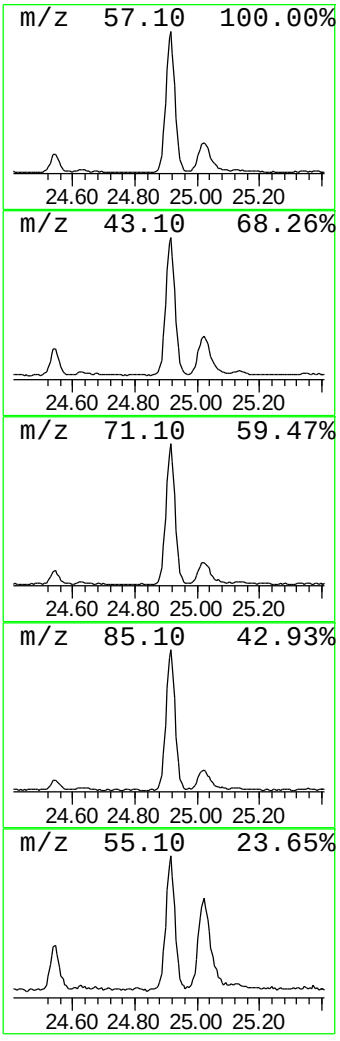
****

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.91	6.11 ng/ul	1258710	Perylene-d12	24.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexatriacontane	507	C36H74	000630-06-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Eicosane, 9-octyl-	394	C28H58	013475-77-9	87
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050218\
Data File : BM014924.D
Acq On : 02 May 2018 15:56
Operator : SJ/JU
Sample : J2631-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AG8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM041918.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
Butane, 2-methoxy...	3.34	30.4	ng/ul	3818220	1	8.49	2510090	20.0
2-Pentanone, 4-hy...	5.48	2.9	ng/ul	363008	1	8.49	2510090	20.0
n-Hexadecanoic acid	18.64	5.5	ng/ul	1211320	4	17.81	4383570	20.0
Octadecanoic acid	19.88	2.5	ng/ul	530997	5	21.90	4222620	20.0
Trichloroacetic a...	21.56	7.1	ng/ul	1492020	5	21.90	4222620	20.0
Oxirane, heptadecyl-	23.24	2.5	ng/ul	518347	6	24.38	4119440	20.0
Heptadecyl heptaf...	23.60	8.9	ng/ul	1826700	6	24.38	4119440	20.0
(DEL) Alkane: Str...	24.91	6.1	ng/ul	1258710	6	24.38	4119440	20.0