LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM030518\
Data File : BM014469.D
Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

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-BM021418.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	3.087	15	17	22	rVB4	25447	31237	1.04%	0.085%
2	3.893	150	154	160	rVB8	28531	50671	1.69%	0.137%
3	4.663	280	285	295	rVB	77397	129217	4.31%	0.350%
4	5.939	498	502	508	rVB4	22254	37747	1.26%	0.102%
5	6.728	630	636	649	rVB	342528	658579	21.98%	1.782%
6	6.863	653	659	667	rBV	301511	480035	16.02%	1.299%
7	7.057	684	692	701	rBV	450296	747747	24.95%	2.023%
8	7.510	762	769	778	rBV	379037	611063	20.39%	1.654%
9	8.251	888	895	907	rBV	446743	865271	28.87%	2.342%
10	8.345	907	911	918	rVB8	20042	44270	1.48%	0.120%
11	8.675	960	967	974	rBV	446933	745105	24.86%	2.016%
12	9.392	1080	1089	1102	rBV	387865	734806	24.52%	1.988%
13	9.698	1133	1141	1150	rBV7	36617	71165	2.37%	0.193%
14	9.945	1176	1183	1203	rBV2	375968	896847	29.93%	2.427%
15	10.286	1234	1241	1249	rBV	458893	802899	26.79%	2.173%
16	10.451	1262	1269	1281	rBV	237948	553728	18.48%	1.498%
17	13.598	1798	1804	1809	rBV	870841	1272864	42.47%	3.444%
18	13.645	1809	1812	1818	rVB2	166073	230280	7.68%	0.623%
19	13.868	1843	1850	1860	rVB	972797	1496504	49.94%	4.050%
20	14.068	1879	1884	1893	rBV3	56460	94235	3.14%	0.255%
21	14.174	1895	1902	1910	rBV2	641042	1039266	34.68%	2.812%
22	14.498	1949	1957	1968	rBV3	145070	442934	14.78%	1.199%
23	14.627	1973	1979	1987	rVV10	50571	130880	4.37%	0.354%
24	14.692	1987	1990	1996	rVV6	23656	43237	1.44%	0.117%
25	14.774	2000	2004	2013	rVB9	17542	42148	1.41%	0.114%
26	15.033	2043	2048	2051	rBV2	75838	97809	3.26%	0.265%
27	15.180	2067	2073	2082	rBV	1146133	1686745	56.28%	4.564%
28	15.362	2099	2104	2111	rBV	291083	482345	16.09%	1.305%
29	15.898	2189	2195	2204	rBV3	73645	133625	4.46%	0.362%
30	16.362	2270	2274	2277	rBV5	31580	47541	1.59%	0.129%
31	16.692	2326	2330	2333	rBV	38132	41382	1.38%	0.112%
32	16.939	2366	2372	2378	rBV	799291	1187573	39.63%	3.214%
33	17.039	2383	2389	2396	rBV2	1152310	1694094	56.53%	4.584%
34	17.327	2433	2438	2442	rBV7	21568	38217	1.28%	0.103%

LSC Area Percent Report

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Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

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-BM021418.M
Title : SVOA CALIBRATION

35	17.850	2520	2527	2536	rBV	855676	1311565	43.76%	3.549%
36	18.133	2570	2575	2576	rBV5	21051	30041	1.00%	0.081%
37	18.156	2576	2579	2584	rVB7	32557	52744	1.76%	0.143%
38	18.268	2595	2598	2602	rVB6	47672	57703	1.93%	0.156%
39	18.521	2637	2641	2647	rBV9	29352	53288	1.78%	0.144%
40	18.933	2709	2711	2715	rVB4	36258	39275	1.31%	0.106%
41	18.992	2718	2721	2722	rBV3	34771	37000	1.23%	0.100%
42	19.021	2723	2726	2728	rVB4	51343	63368	2.11%	0.171%
43	19.144	2741	2747	2760	rBV	1668116	2684325	89.57%	7.264%
44	19.350	2777	2782	2794	rBV	1272715	1801405	60.11%	4.875%
45	19.586	2818	2822	2830	rVB	312016	405518	13.53%	1.097%
46	19.874	2867	2871	2873	rBV3	104692	132748	4.43%	0.359%
47	20.291	2939	2942	2947	rVB5	69003	89001	2.97%	0.241%
48	20.862	3035	3039	3048	rBV	2524218	2996864	100.00%	8.110%
49	20.938	3049	3052	3056	rBV2	278139	318743	10.64%	0.863%
50	21.156	3084	3089	3094	rBV	924187	1299357	43.36%	3.516%
51	21.744	3185	3189	3197	rVB	1816331	2783525	92.88%	7.532%
52	21.815	3198	3201	3205	rVB	325784	382786	12.77%	1.036%
53	22.709	3348	3353	3358	rVB2	460184	729632	24.35%	1.974%
54	23.203	3432	3437	3444	rVB2	817782	1400420	46.73%	3.790%
55	23.344	3456	3461	3468	rVB2	501509	881691	29.42%	2.386%
56	26.362	3968	3974	3985	rVB6	619721	1740593	58.08%	4.710%

Sum of corrected areas: 36953658

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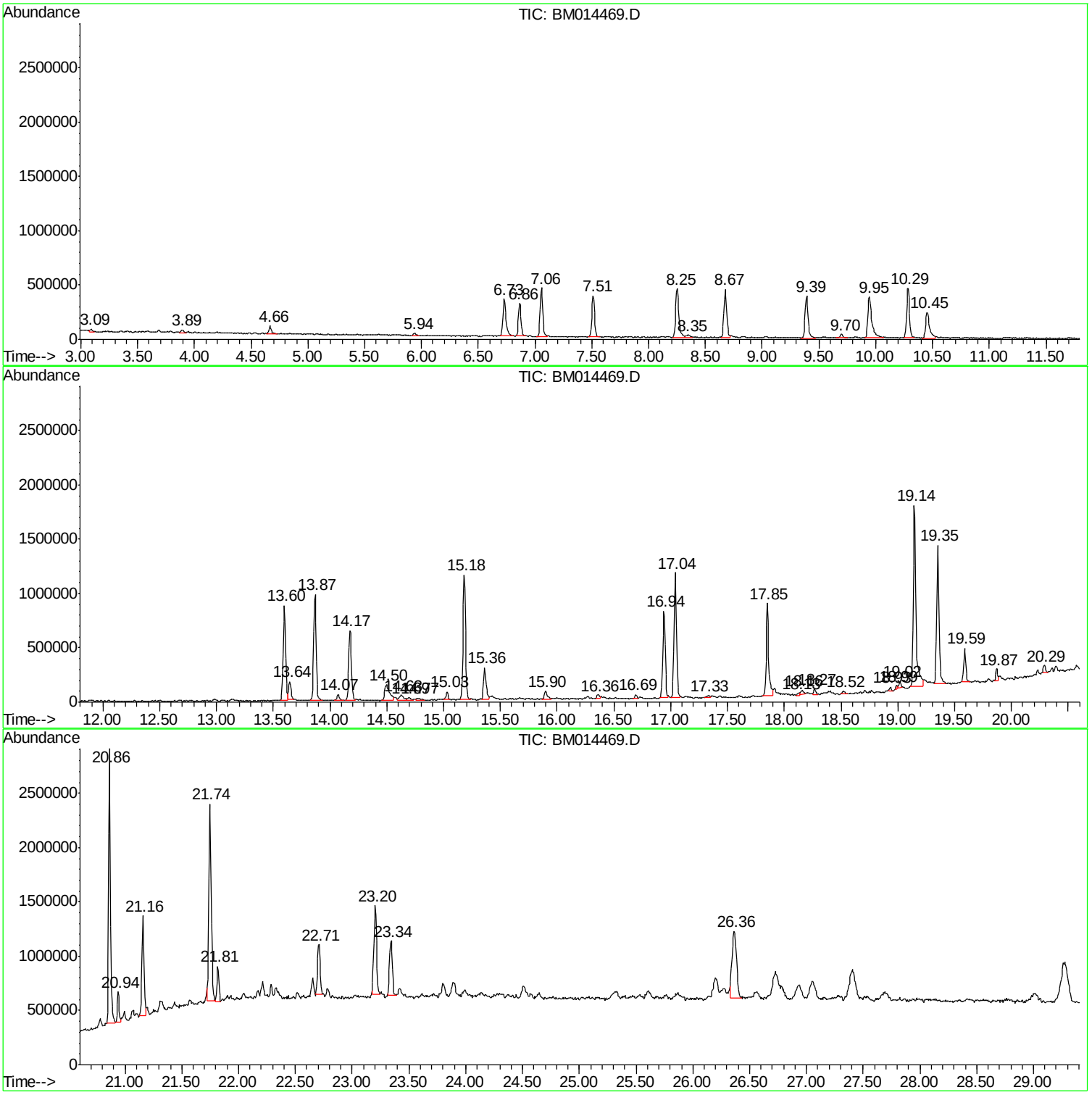
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

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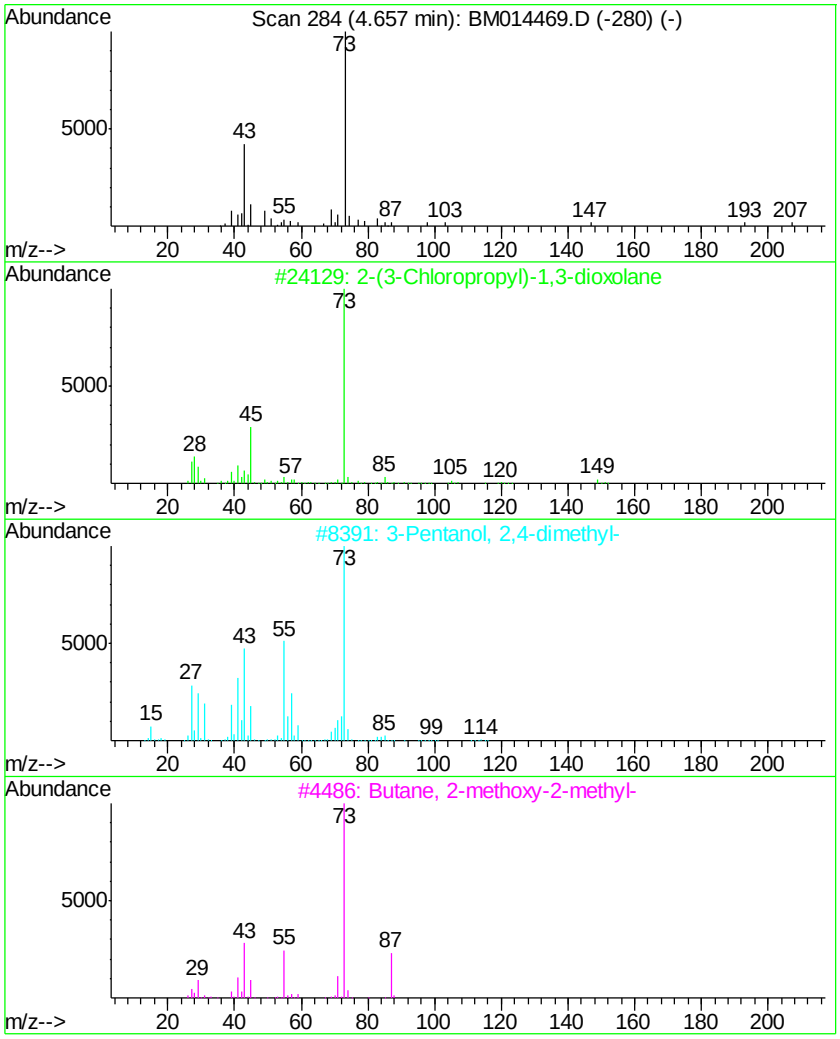
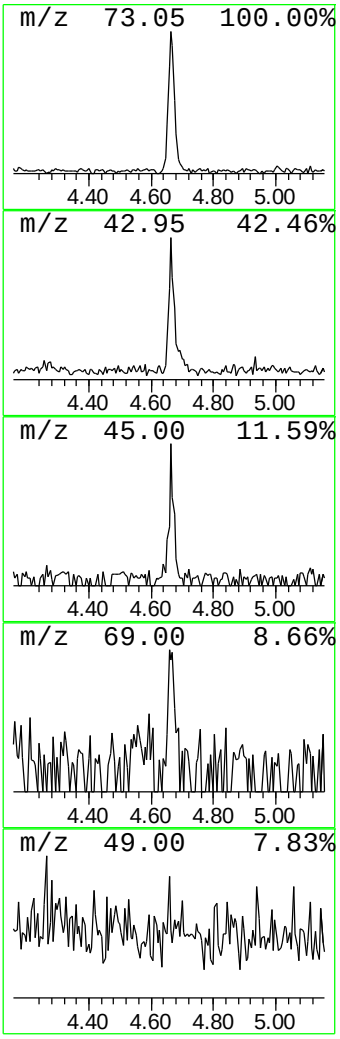
****

Peak Number 1 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	4.23 ng/ul	129217	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3-Chloropropyl)-1,3-dioxolane	150	C6H11ClO2	016686-11-6	47
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	36
3	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	28
4	1H-Cyclopenta[c]furan-3(3aH)-one...	196	C10H12O4	1000141-74-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	23





Data Path : Z:\HPCHEM1\BNA M\DATA\BM030518\
Data File : BM014469.D
Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

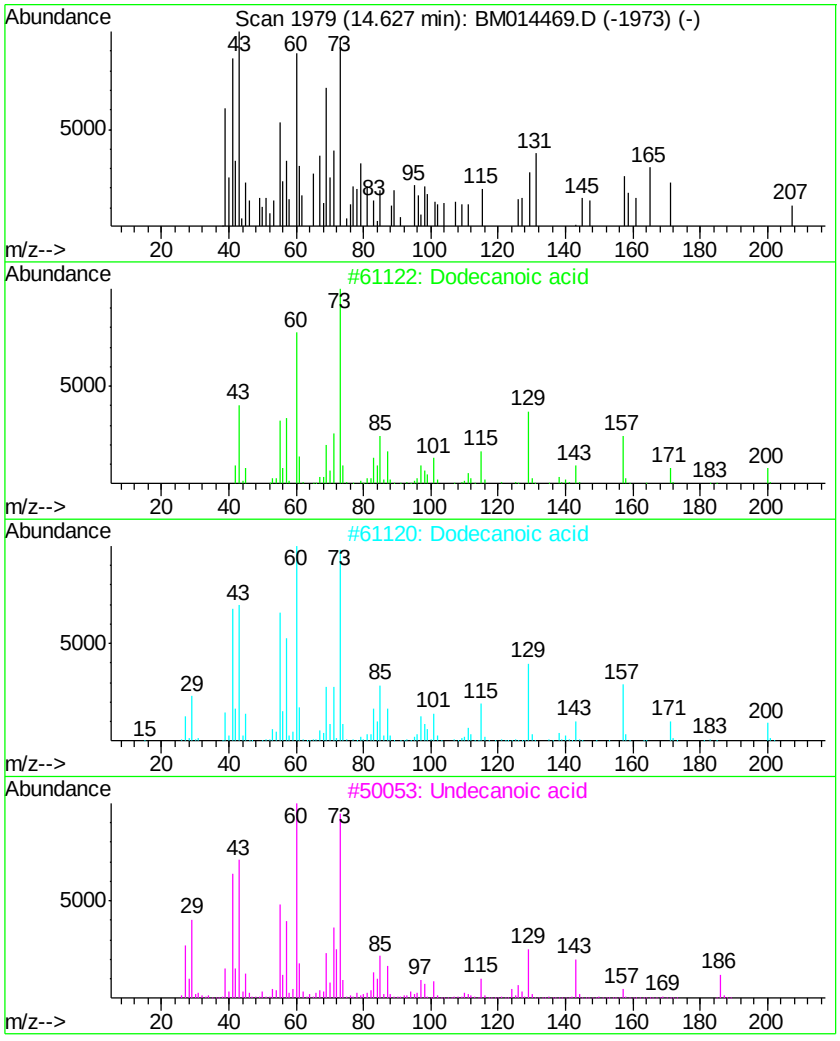
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

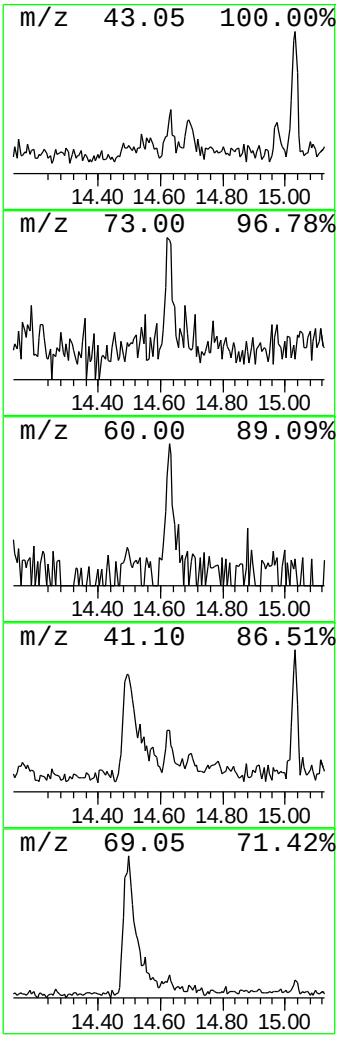
****

Peak Number 2 unknown-02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.52 ng/ul	130880	Acenaphthene-d10	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	32
2	Dodecanoic acid	200	C12H24O2	000143-07-7	32
3	Undecanoic acid	186	C11H22O2	000112-37-8	25
4	Nonanoic acid	158	C9H18O2	000112-05-0	25
5	n-Decanoic acid	172	C10H20O2	000334-48-5	16





Library Search Compound Report

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Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

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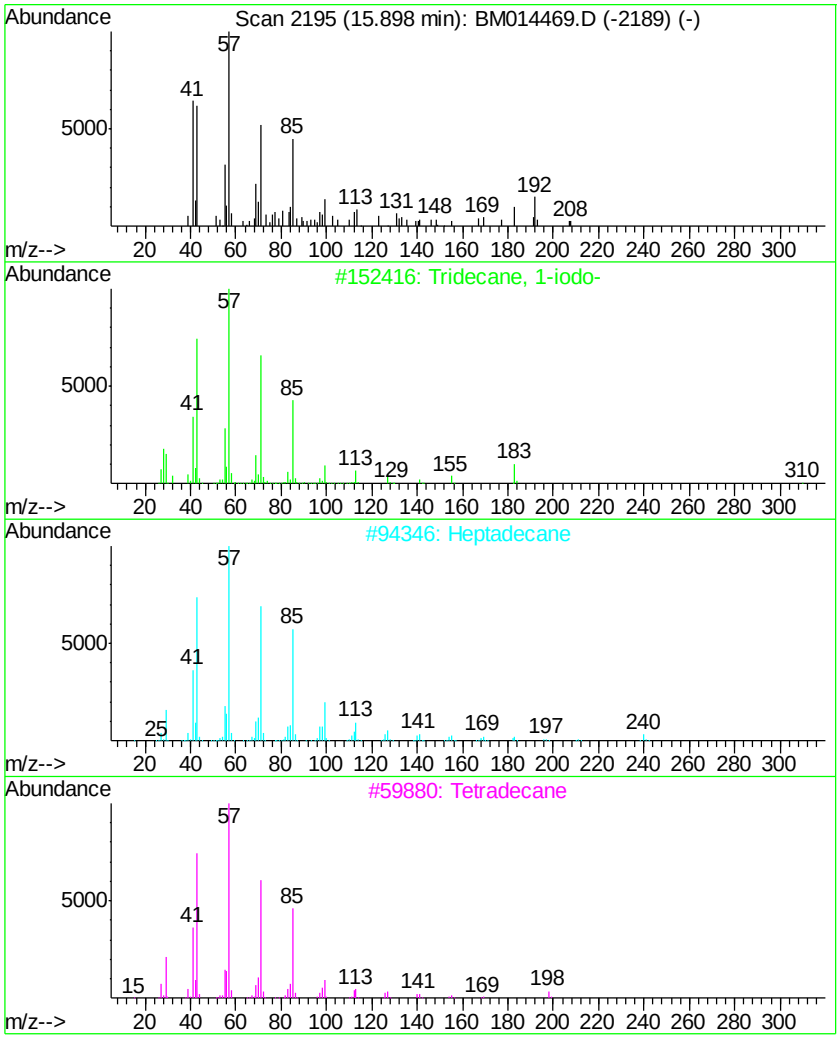
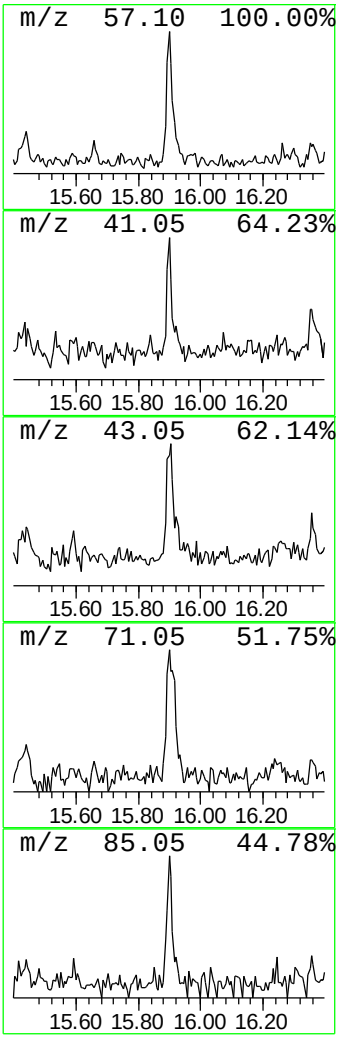
Peak Number 3 Tridecane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	2.25 ng/ul	133625	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
2	Heptadecane	240	C17H36	000629-78-7	64
3	Tetradecane	198	C14H30	000629-59-4	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Octacosane	394	C28H58	000630-02-4	64





Library Search Compound Report

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Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

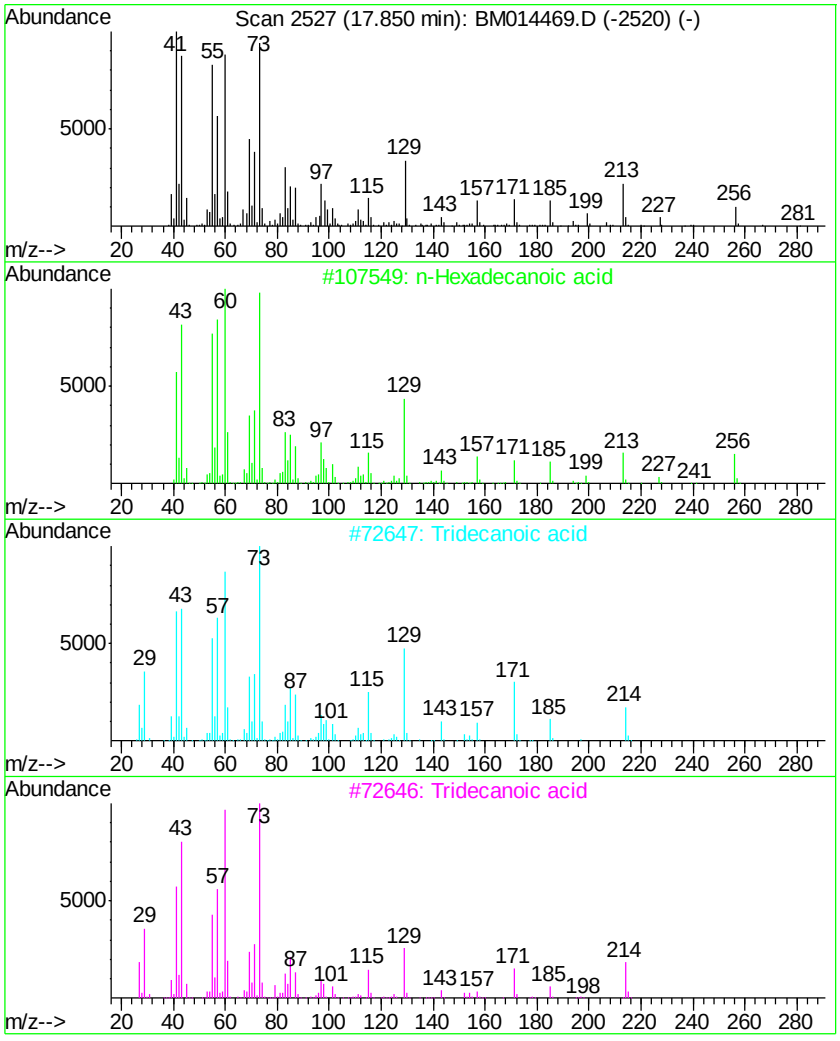
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

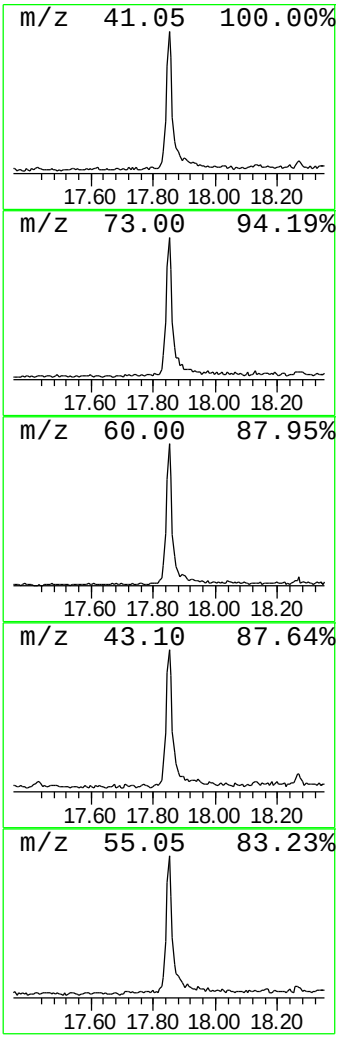
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	22.09 ng/ul	1311570	Phenanthrene-d10	16.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





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Misc :
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Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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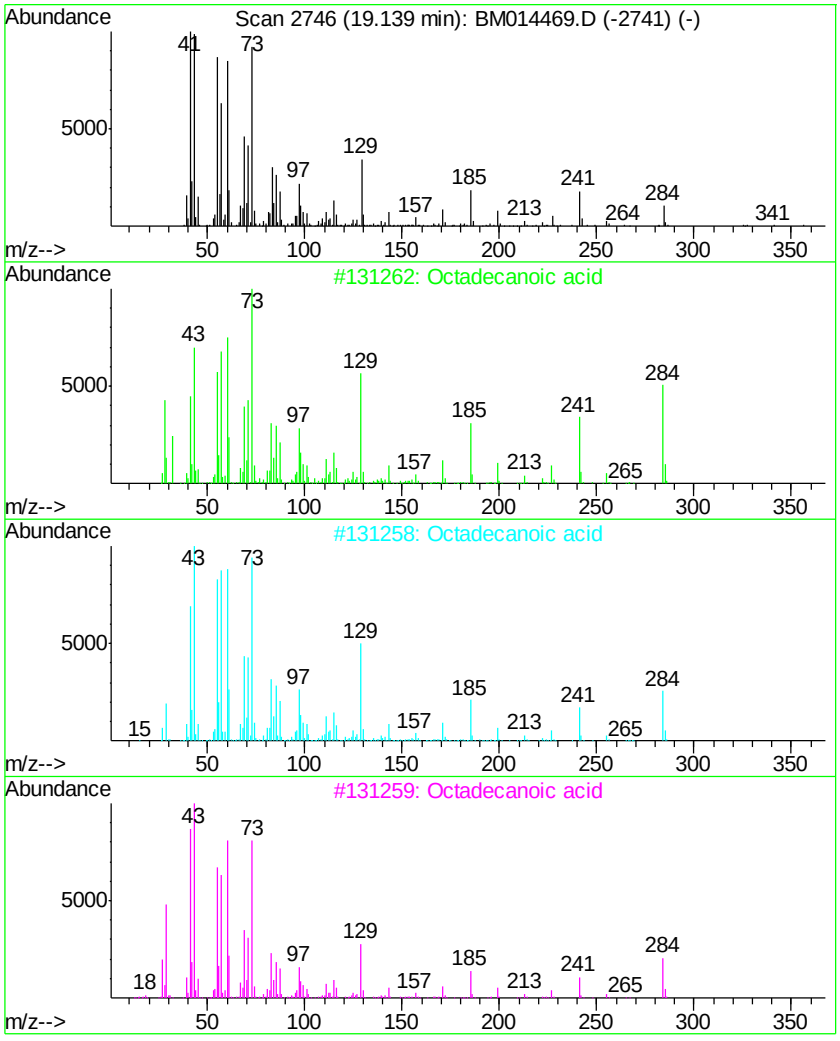
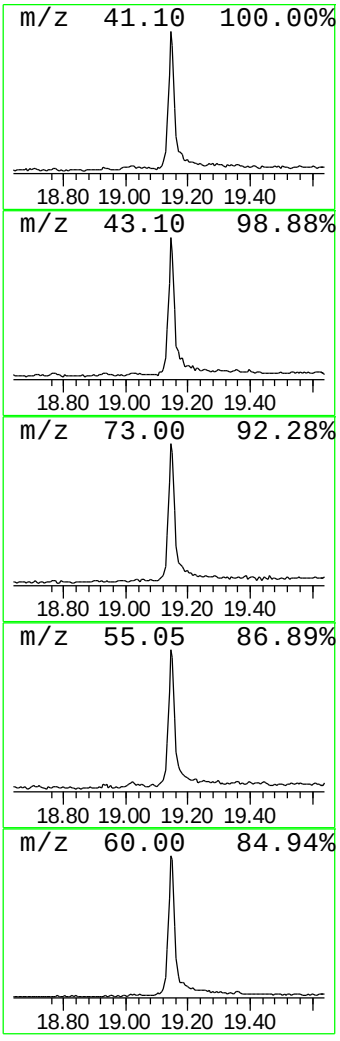
Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	41.32 ng/ul	2684330	Chrysene-d12	21.16

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	96
4	Octadecanoic acid	284	C18H36O2	000057-11-4	95
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





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Quant Title : SVOA CALIBRATION

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

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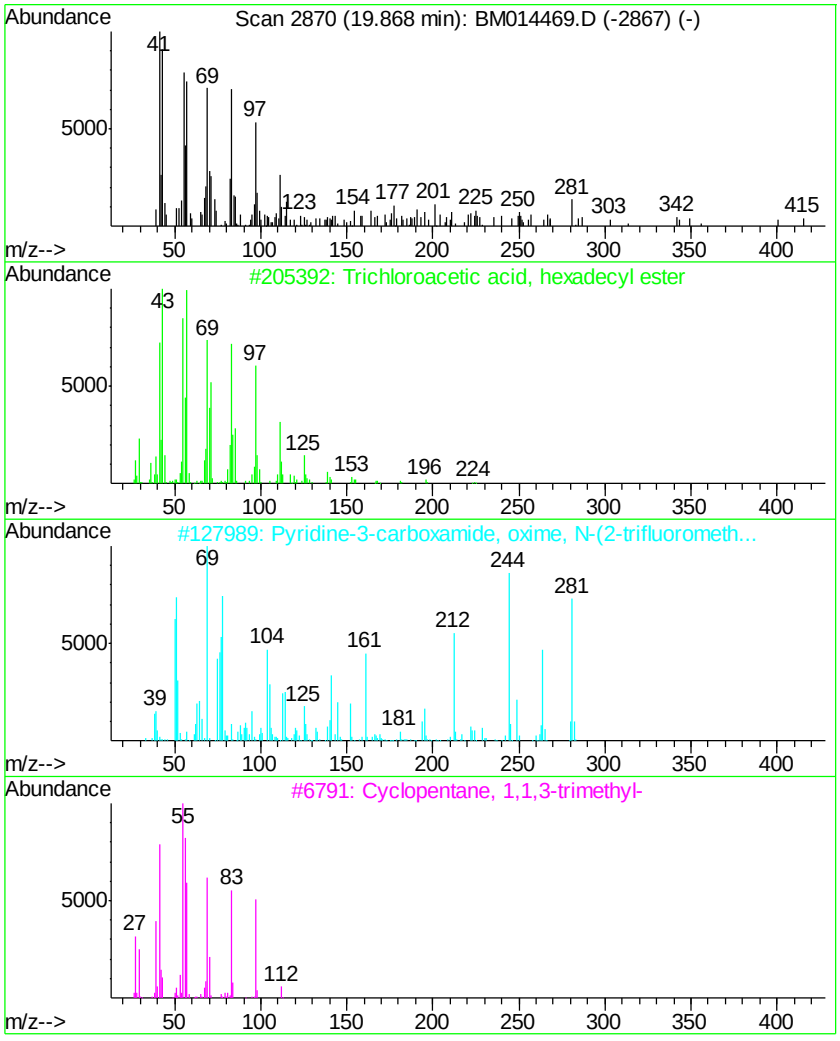
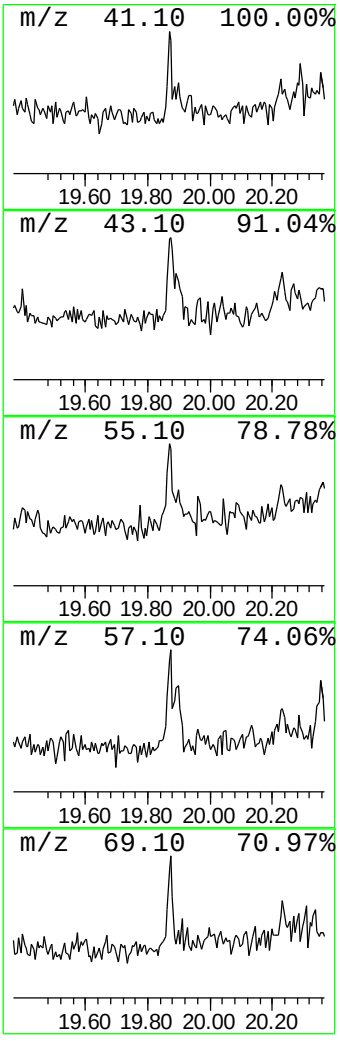
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	2.04 ng/ul	132748	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	72
2	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	53
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	53
4	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	52
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	49





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Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

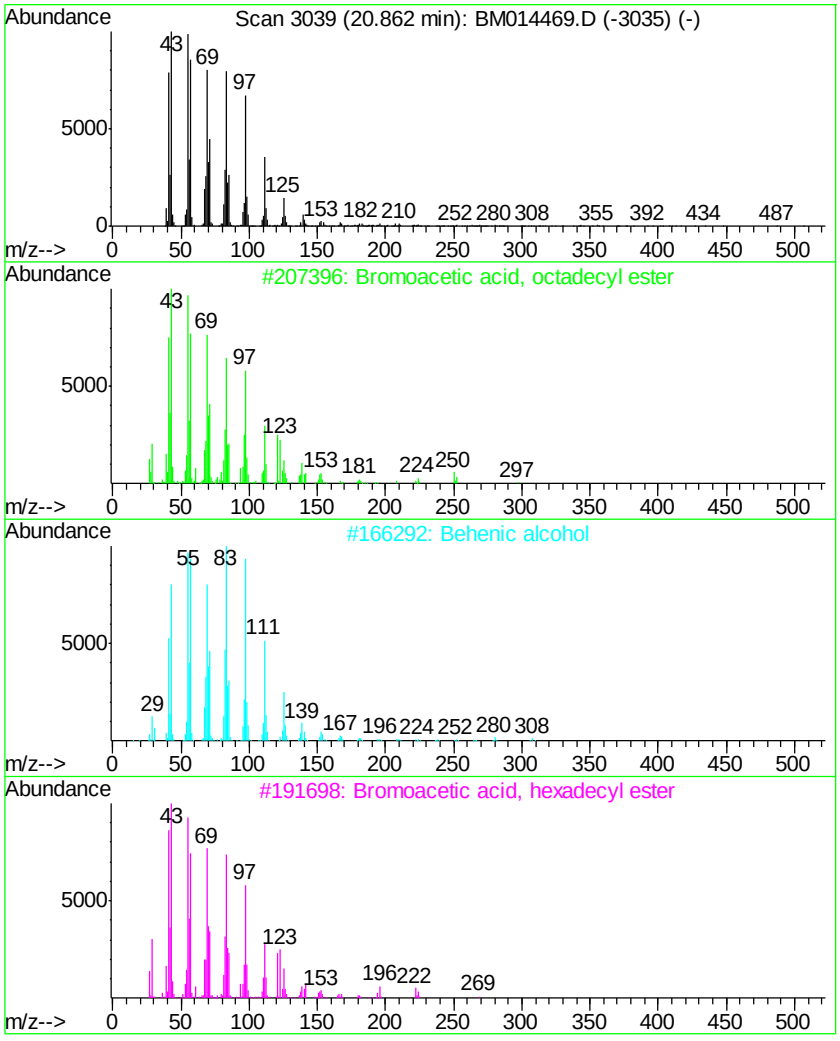
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

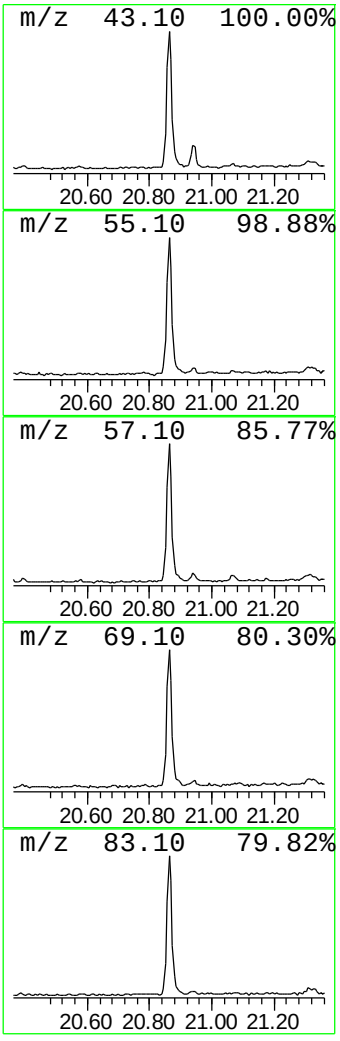
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	46.13 ng/ul	2996860	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
5	1-Hexadecanol	242	C16H34O	036653-82-4	87





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Data File : BM014469.D
Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

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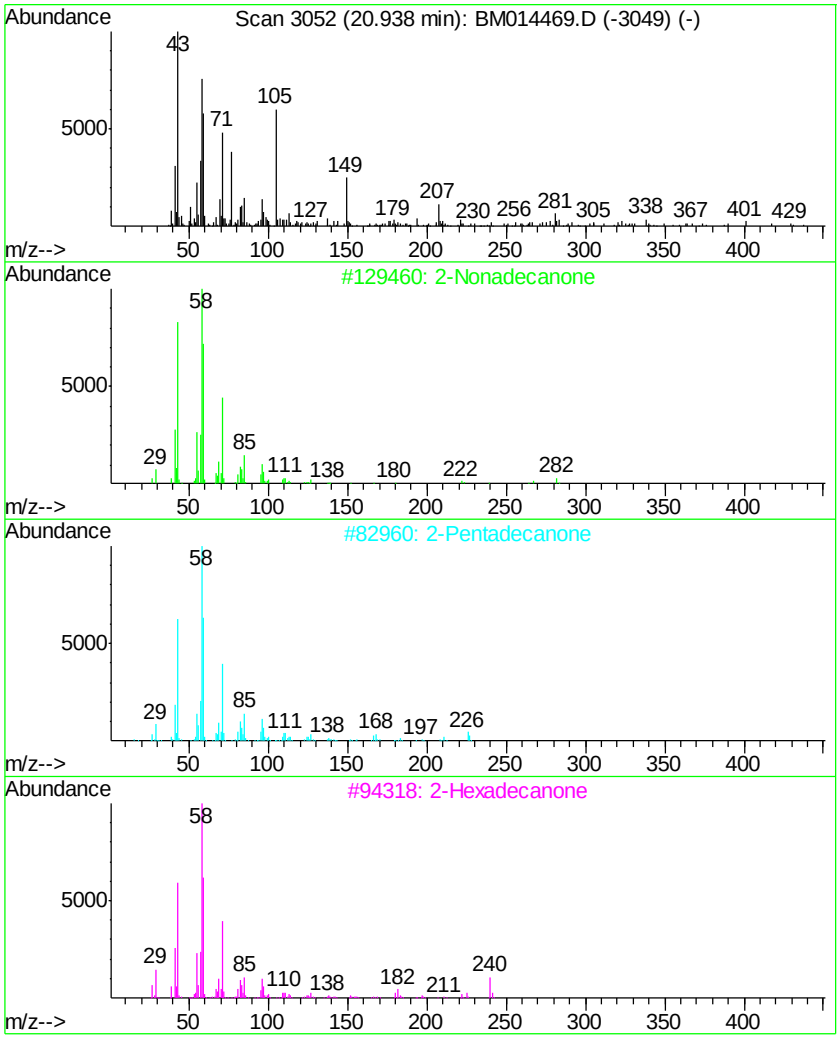
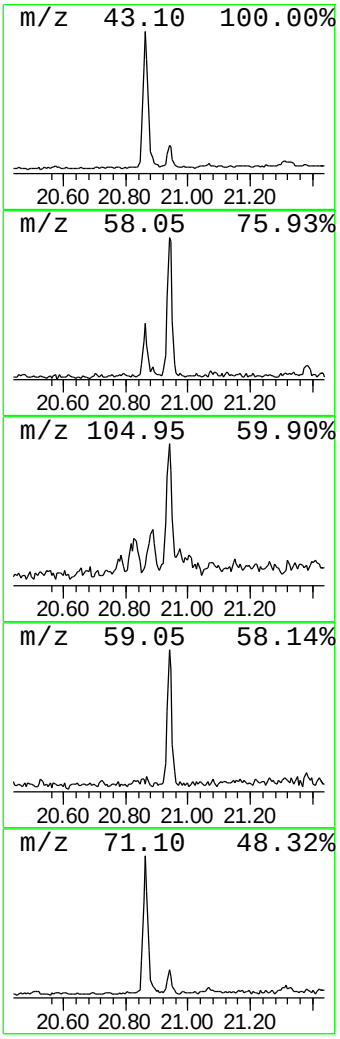
Peak Number 9 2-Nonadecanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	4.91 ng/ul	318743	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone	282	C19H38O	000629-66-3	55
2	2-Pentadecanone	226	C15H30O	002345-28-0	43
3	2-Hexadecanone	240	C16H32O	018787-63-8	43
4	O-Methyl S-2-dimethylaminoethyl ...	211	C7H18NO2PS	1000226-15-4	38
5	2-Tetradecanone	212	C14H28O	002345-27-9	38





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Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

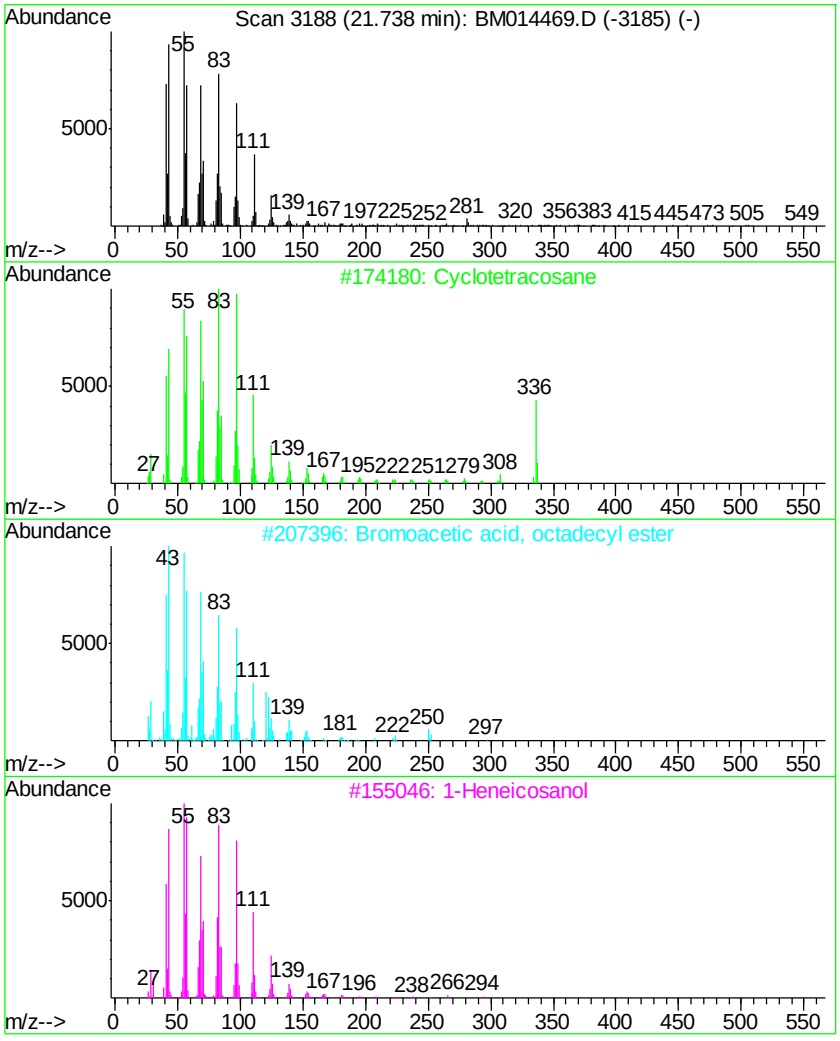
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

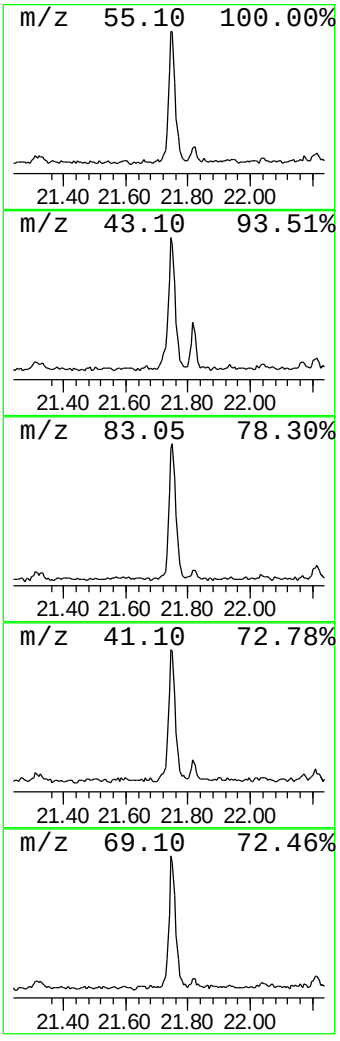
****

Peak Number 10 (DEL) Alkane: Cyclic21.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	42.84 ng/ul	2783530	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	90
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	81
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	81





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Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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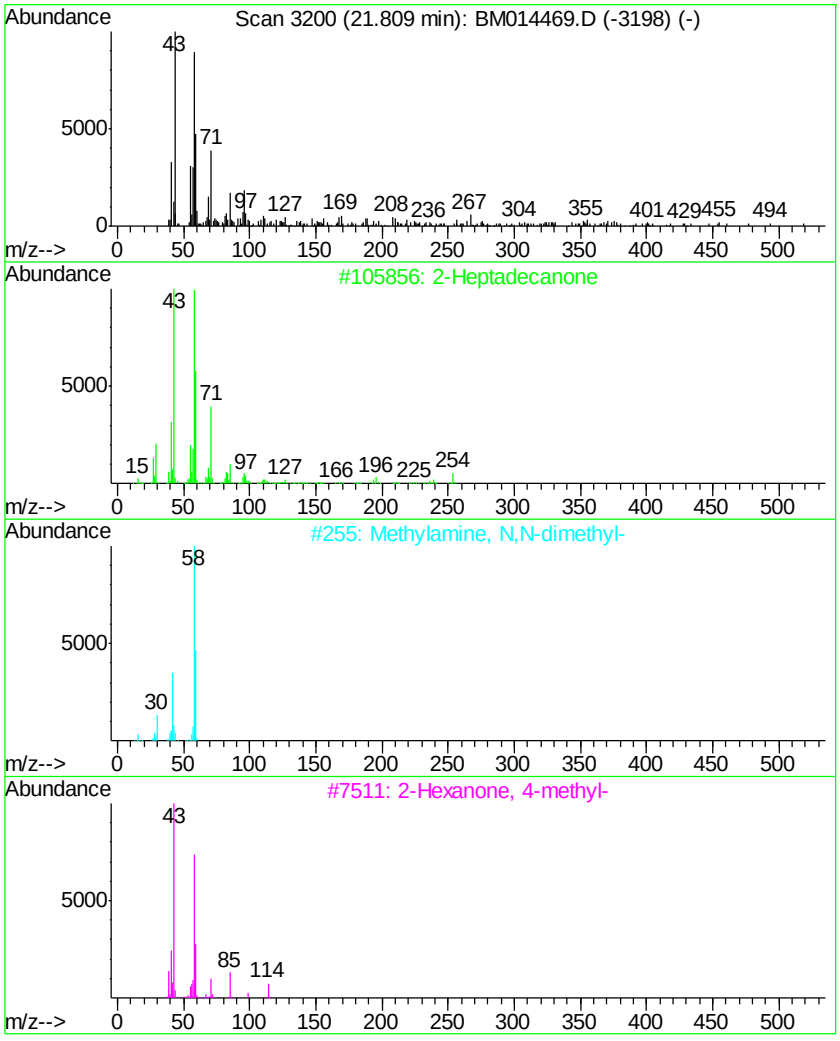
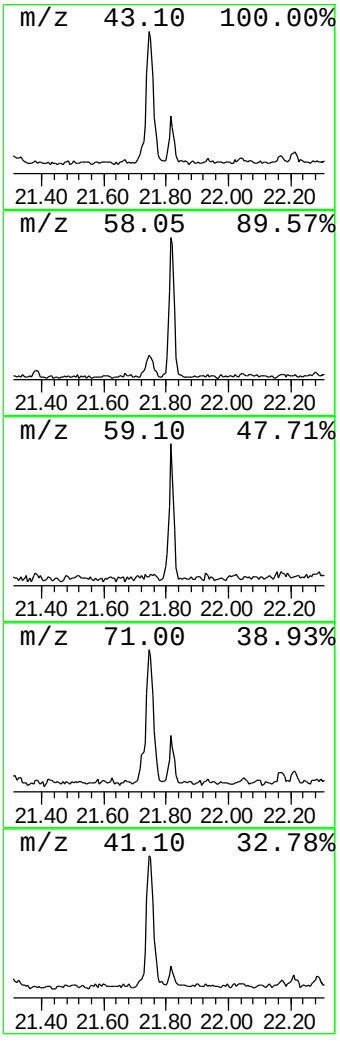
Peak Number 11 2-Heptadecanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	5.89 ng/ul	382786	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptadecanone	254	C17H34O	002922-51-2	78
2	Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	50
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	47
4	2-Nonanone	142	C9H18O	000821-55-6	43
5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	43





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Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

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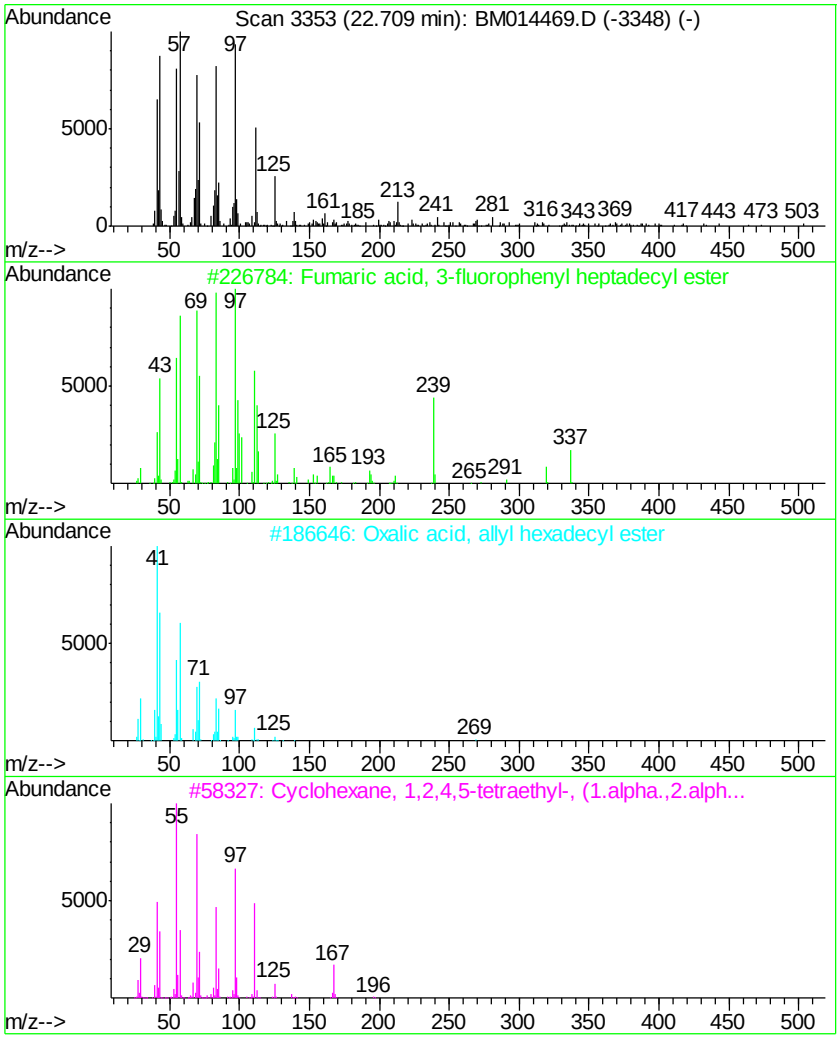
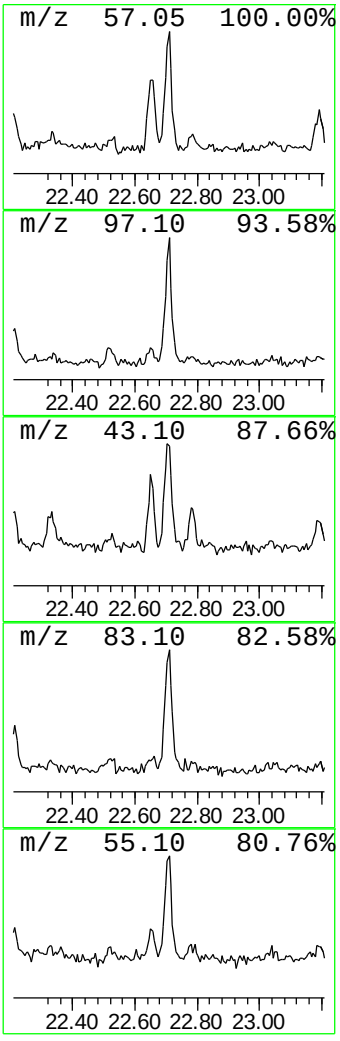
Peak Number 12 Fumaric acid, 3-fluoropheny... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.71	16.55 ng/ul	729632	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 3-fluorophenyl hep...	448	C27H41FO4	1000345-21-3	86
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	64
3	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	46
4	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	42
5	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	38





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Data File : BM014469.D
Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

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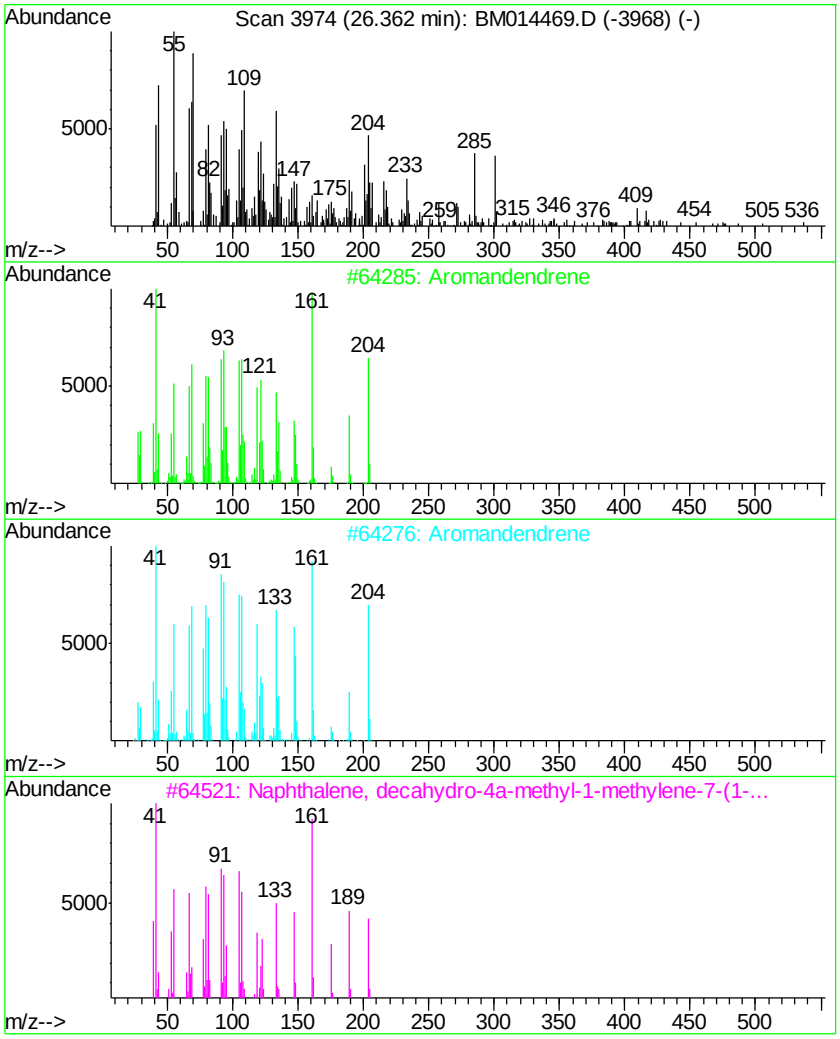
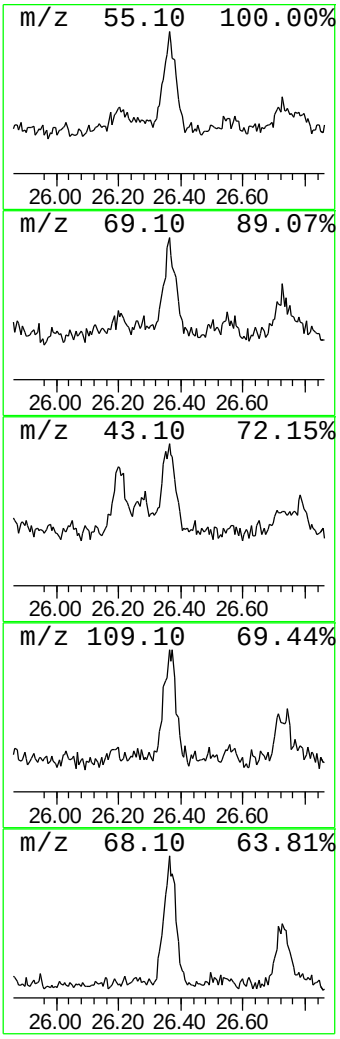
Peak Number 13 Aromandendrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.36	39.48 ng/ul	1740590	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aromandendrene	204	C15H24	000489-39-4	81
2	Aromandendrene	204	C15H24	000489-39-4	41
3	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	41
4	3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	41
5	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM030518\
Data File : BM014469.D
Acq On : 05 Mar 2018 12:47
Operator : SJ/JU
Sample : J1631-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BE603

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.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	4.66	4.2	ng/ul	129217	1	7.51	611063	20.0
unknown-02	14.63	2.5	ng/ul	130880	3	14.17	1039270	20.0
Tridecane, 1-iodo-	15.90	2.3	ng/ul	133625	4	16.94	1187570	20.0
n-Hexadecanoic acid	17.85	22.1	ng/ul	1311570	4	16.94	1187570	20.0
Octadecanoic acid	19.14	41.3	ng/ul	2684330	5	21.16	1299360	20.0
Trichloroacetic a...	19.87	2.0	ng/ul	132748	5	21.16	1299360	20.0
Bromoacetic acid,...	20.86	46.1	ng/ul	2996860	5	21.16	1299360	20.0
2-Nonadecanone	20.94	4.9	ng/ul	318743	5	21.16	1299360	20.0
(DEL) Alkane: Cyc...	21.74	42.8	ng/ul	2783530	5	21.16	1299360	20.0
2-Heptadecanone	21.81	5.9	ng/ul	382786	5	21.16	1299360	20.0
Fumaric acid, 3-f...	22.71	16.6	ng/ul	729632	6	23.34	881691	20.0
Aromandendrene	26.36	39.5	ng/ul	1740590	6	23.34	881691	20.0