LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120319\
Data File : BM023984.D
Acq On : 03 Dec 2019 23:49
Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

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-BM112719MA.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	3.034	22	25	32	rVB	41410	59272	0.15%	0.041%
2	3.652	126	130	135	rVB2	40009	58438	0.15%	0.041%
3	4.646	294	299	306	rBV	41195	74295	0.19%	0.052%
4	6.675	637	644	659	rBV	745270	1358226	3.53%	0.943%
5	6.834	665	671	687	rVB	571420	982448	2.55%	0.682%
6	7.016	696	702	716	rVB	809900	1334603	3.47%	0.926%
7	7.481	774	781	791	rBV	1086711	1709986	4.44%	1.187%
8	8.198	895	903	912	rBV	941127	1573224	4.09%	1.092%
9	8.316	919	923	927	rVB	28693	45746	0.12%	0.032%
10	8.634	969	977	993	rBV	689403	1187477	3.09%	0.824%
11	9.351	1092	1099	1108	rBV	546081	935021	2.43%	0.649%
12	9.887	1182	1190	1203	rBV	872676	1623574	4.22%	1.127%
13	10.251	1243	1252	1264	rBV	1463785	2419489	6.29%	1.680%
14	10.404	1271	1278	1296	rBV	367254	865608	2.25%	0.601%
15	13.563	1808	1815	1819	rBV	1569491	2170560	5.64%	1.507%
16	13.610	1819	1823	1832	rVB	713732	1040001	2.70%	0.722%
17	13.827	1854	1860	1874	rBV	1890478	2820114	7.33%	1.958%
18	14.139	1906	1913	1924	rBV	2087068	3119281	8.11%	2.165%
19	14.380	1947	1954	1973	rBV	360956	842536	2.19%	0.585%
20	14.539	1976	1981	1985	rVV5	40271	85118	0.22%	0.059%
21	14.592	1985	1990	2001	rVB6	66398	135504	0.35%	0.094%
22	15.145	2077	2084	2094	rBV	2402514	3547517	9.22%	2.463%
23	15.286	2102	2108	2121	rBV	473538	706020	1.83%	0.490%
24	15.386	2121	2125	2130	rVB4	26430	39014	0.10%	0.027%
25	16.898	2376	2382	2391	rBV	2567117	3572874	9.29%	2.480%
26	16.992	2392	2398	2409	rBV2	2501784	3647799	9.48%	2.532%
27	17.821	2534	2539	2547	rBV	236024	379182	0.99%	0.263%
28	19.133	2755	2762	2768	rBV5	137629	318910	0.83%	0.221%
29	19.186	2768	2771	2777	rVB2	32568	53829	0.14%	0.037%
30	19.298	2785	2790	2797	rBV	3324840	4544978	11.81%	3.155%
31	19.886	2887	2890	2896	rVB2	80046	89566	0.23%	0.062%
32	20.756	3034	3038	3044	rBV2	232894	327670	0.85%	0.227%
33	20.845	3049	3053	3060	rBV	939554	1205130	3.13%	0.837%
34	20.962	3071	3073	3078	rVB5	110428	148189	0.39%	0.103%

LSC Area Percent Report

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Misc :
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Instrument : BNA_M
ClientSampleId : JLNT0

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-BM112719MA.M
Title : SVOA CALIBRATION

35	21.103	3092	3097	3105	rBV	3539626	4409420	11.46%	3.061%
36	21.321	3131	3134	3137	rVB2	117934	122927	0.32%	0.085%
37	21.498	3161	3164	3169	rBV5	172626	233802	0.61%	0.162%
38	21.703	3195	3199	3207	rBV	1714847	2431374	6.32%	1.688%
39	22.150	3272	3275	3278	rBV	183816	189026	0.49%	0.131%
40	22.192	3278	3282	3287	rBV	1024147	1201482	3.12%	0.834%
41	22.633	3353	3357	3361	rVB	567696	739851	1.92%	0.514%
42	22.680	3362	3365	3373	rVB2	362079	587962	1.53%	0.408%
43	23.109	3432	3438	3444	rBV	2970512	5200481	13.52%	3.610%
44	23.244	3454	3461	3473	rVB	2985962	5977240	15.53%	4.149%
45	23.533	3506	3510	3514	rBV	450956	748331	1.94%	0.519%
46	26.497	4001	4014	4021	rBV	12396385	38477649	100.00%	26.710%
47	26.574	4021	4027	4037	rVB	3757407	10359344	26.92%	7.191%
48	26.827	4061	4070	4082	rBV2	2745212	9932365	25.81%	6.895%
49	26.974	4086	4095	4115	rVB4	4579719	17128725	44.52%	11.890%
50	28.732	4387	4394	4403	rBV	1087145	3297425	8.57%	2.289%

Sum of corrected areas: 144058603

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Instrument : BNA_M
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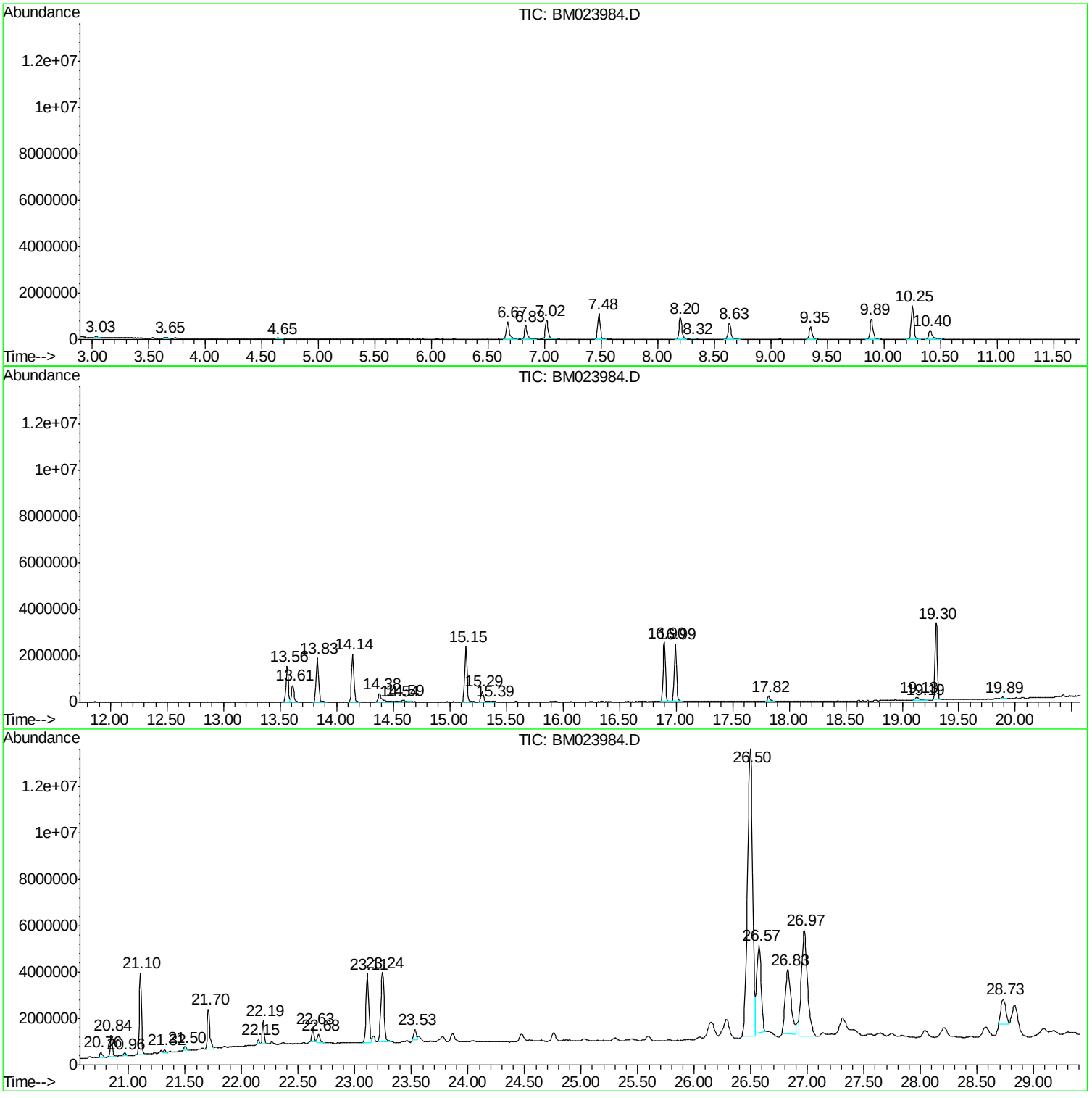
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

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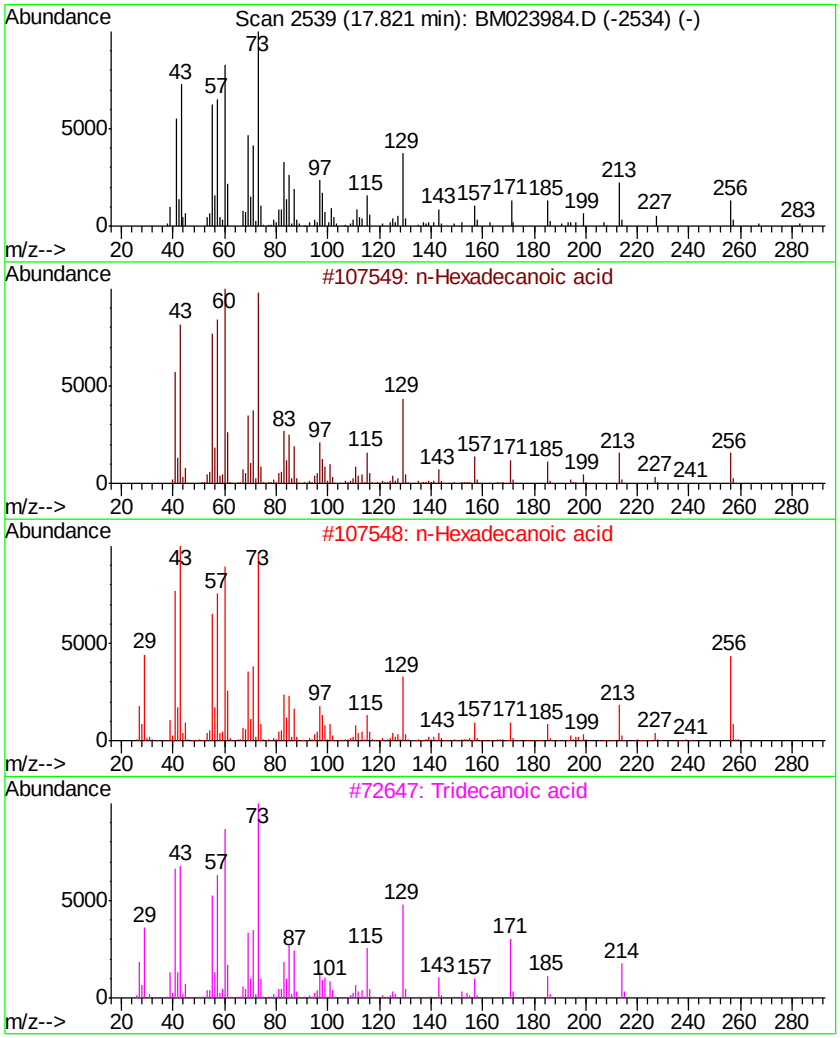
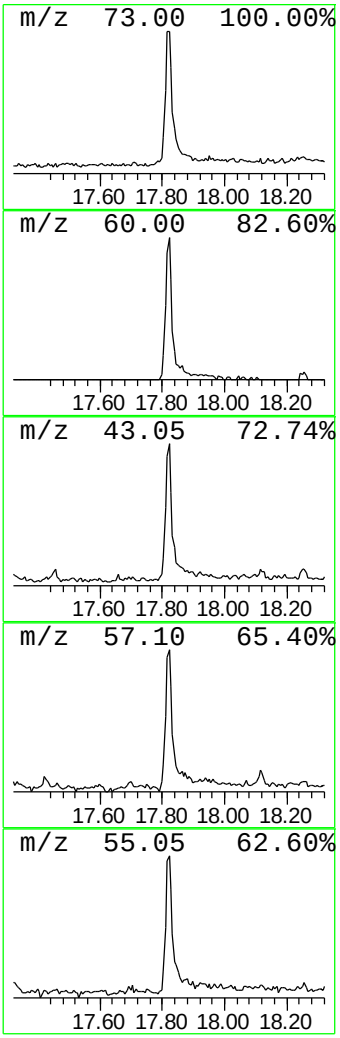
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	2.12 ng/ul	379182	Phenanthrene-d10	16.90

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	99
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	83





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Instrument : BNA_M
ClientSampleId : JLNT0

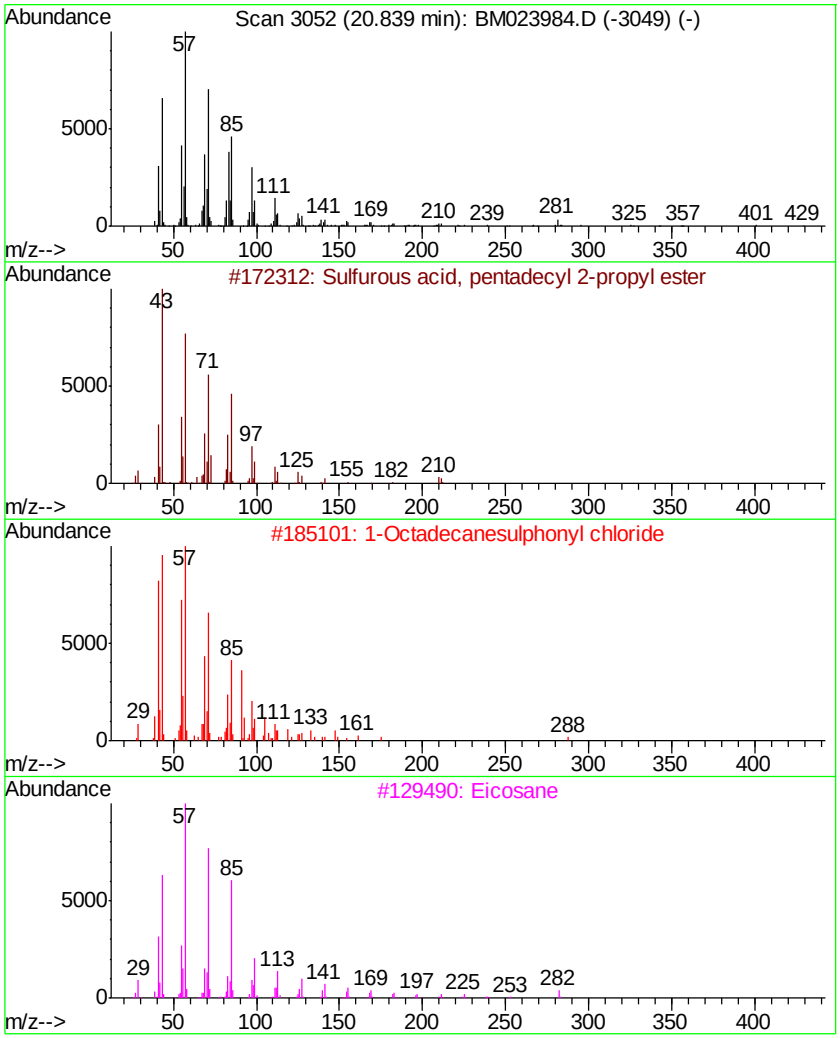
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

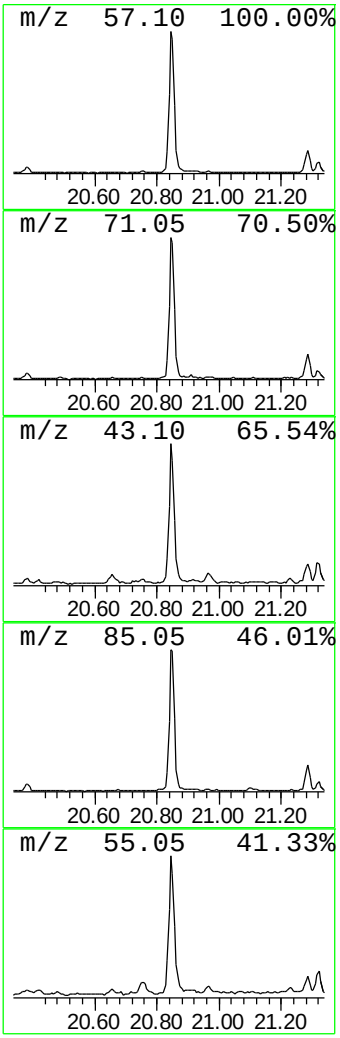
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfurous acid, pentadecyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	5.47 ng/ul	1205130	Chrysene-d12	21.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
3	Eicosane	282	C20H42	000112-95-8	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

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Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

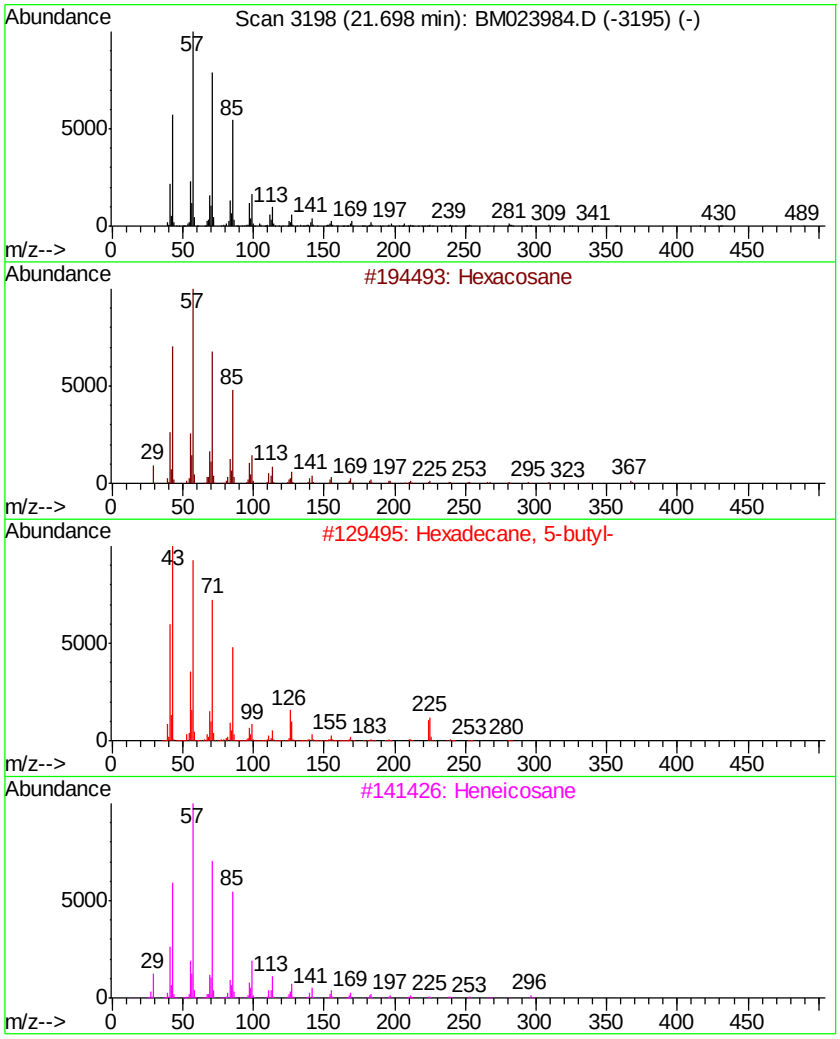
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

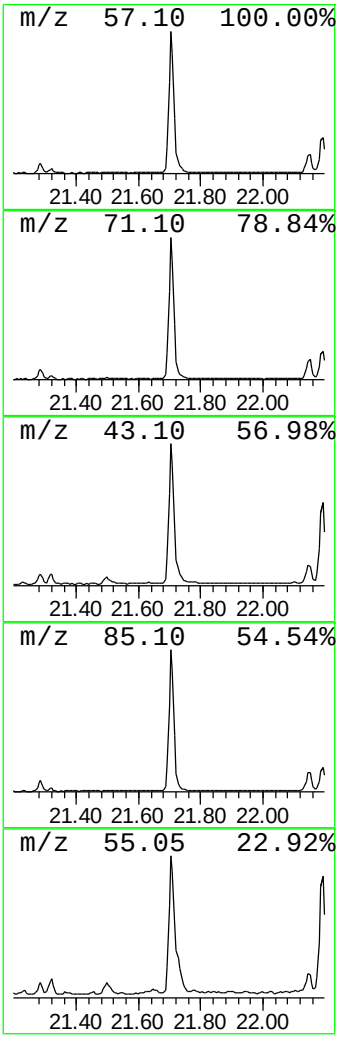
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	11.03 ng/ul	2431370	Chrysene-d12	21.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptacosane	380	C27H56	000593-49-7	87





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Quant Title : SVOA CALIBRATION

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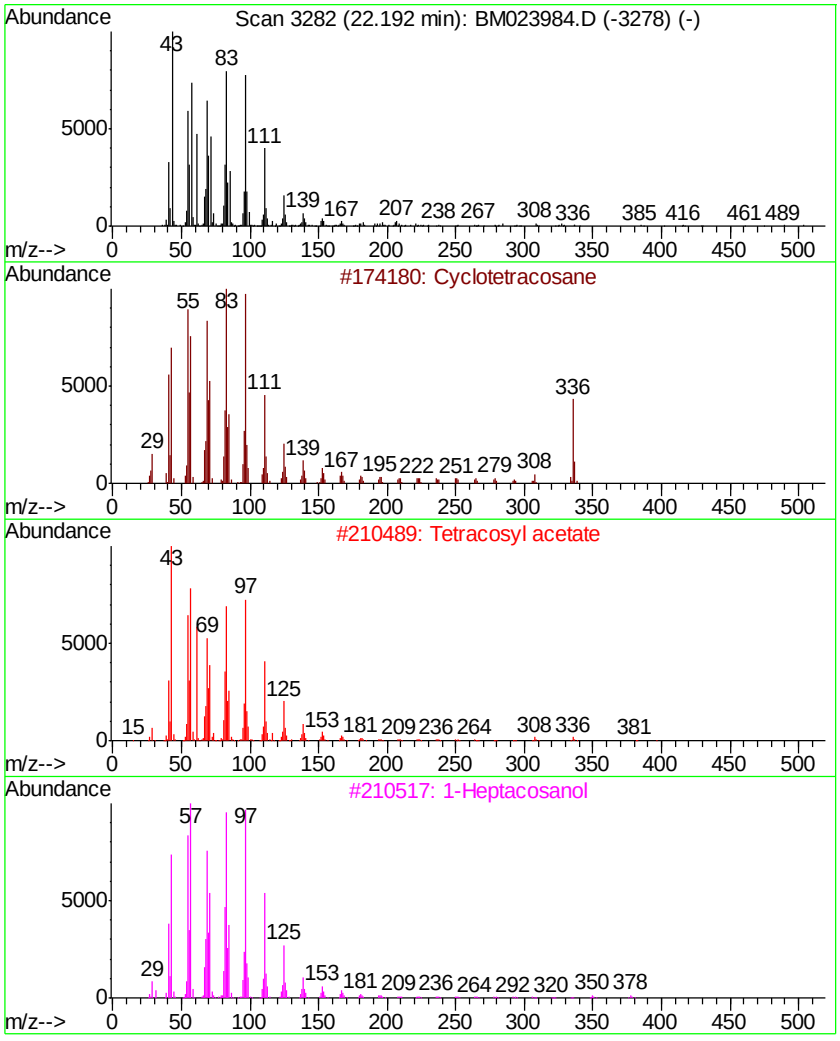
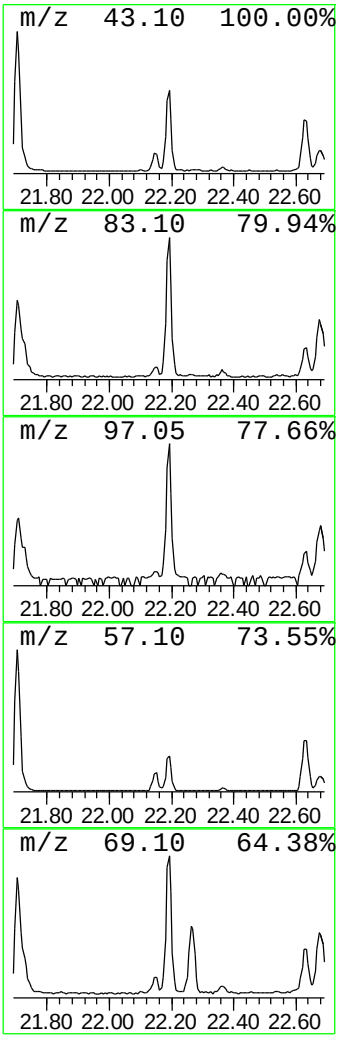
****

Peak Number 4 (DEL) Alkane: Cyclic22.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.19	4.02 ng/ul	1201480	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	Tetracosyl acetate	396	C26H52O2	1000351-78-1	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Tricosyl acetate	382	C25H50O2	1000351-77-8	93
5	1-Docosanol, acetate	368	C24H48O2	000822-26-4	93





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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

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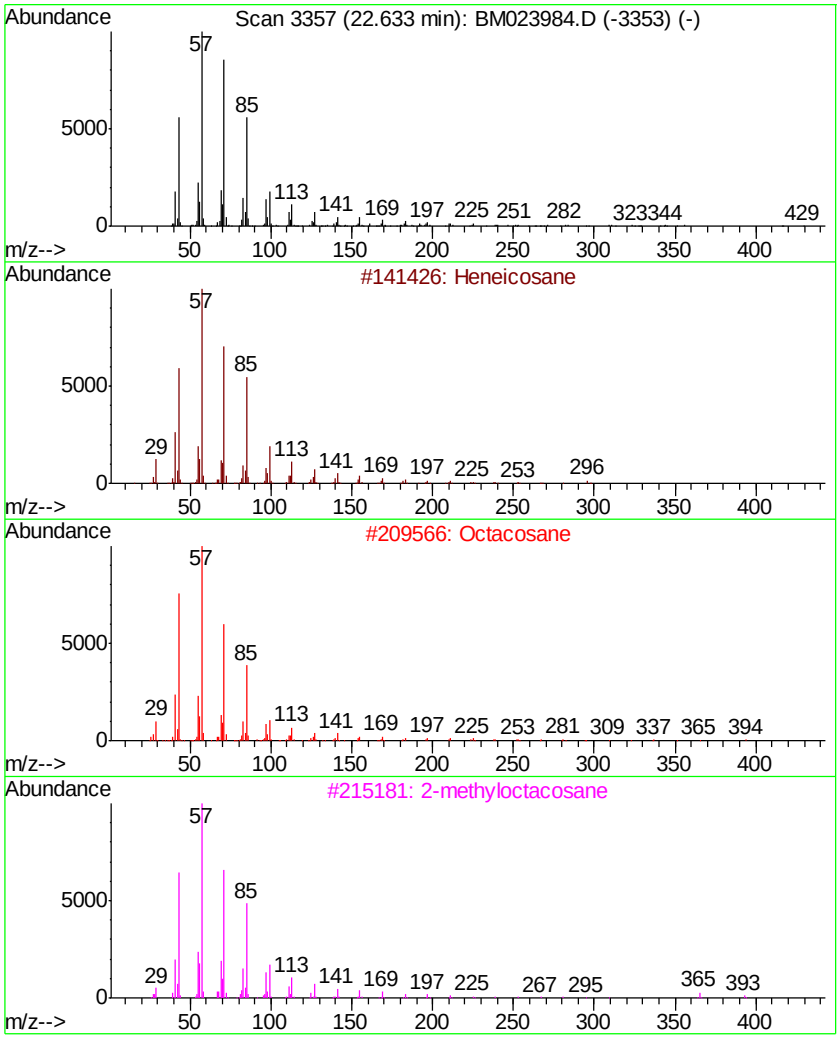
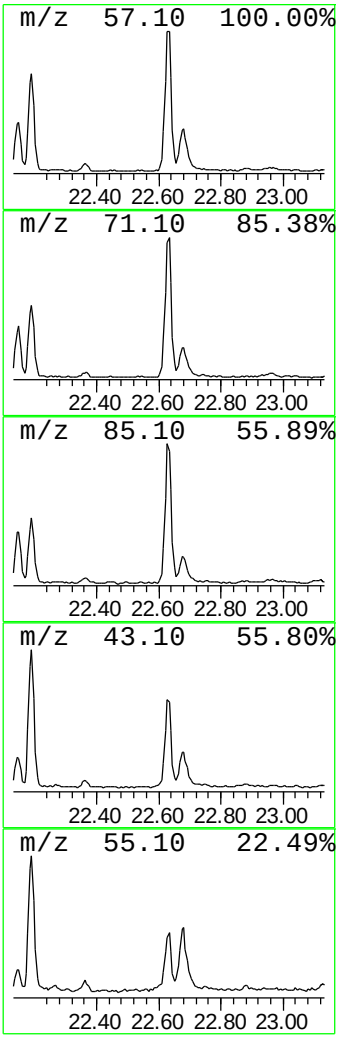
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.48 ng/ul	739851	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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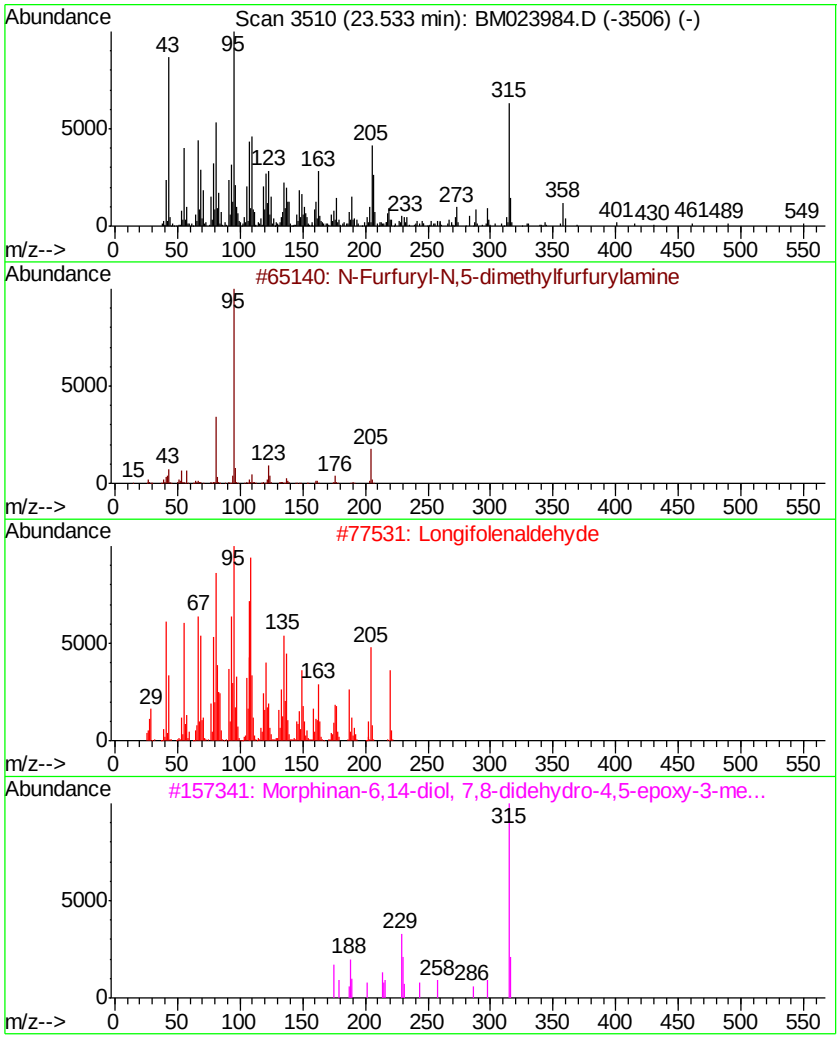
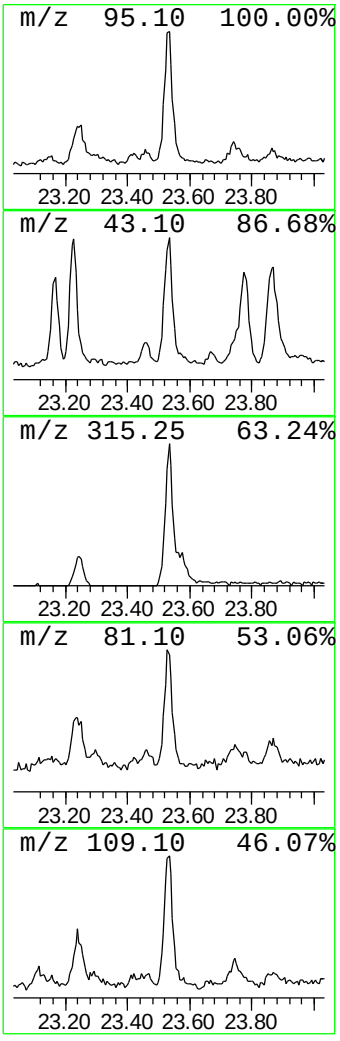
Peak Number 6 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.53	2.50 ng/ul	748331	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Furfuryl-N,5-dimethylfurfurvla...	205	C12H15NO2	1000245-11-0	27
2	Longifolenaldehyde	220	C15H24O	019890-84-7	17
3	Morphinan-6,14-diol, 7,8-didehyd...	315	C18H21NO4	004829-46-3	12
4	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	10
5	Isophthalic acid, butyl 3,7-dime...	360	C22H32O4	1000356-73-8	10





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Quant Title : SVOA CALIBRATION

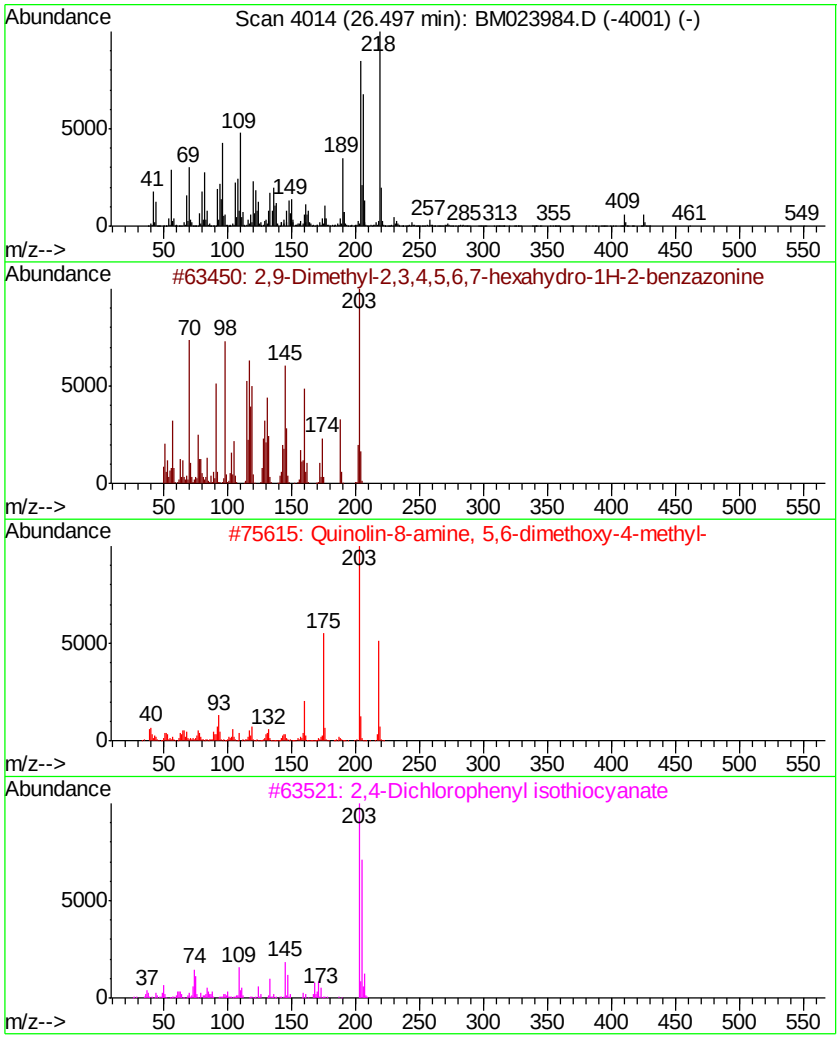
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

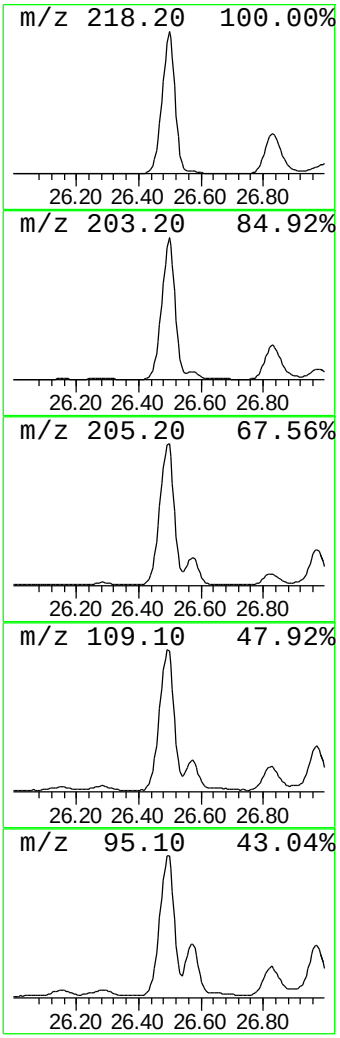
****

Peak Number 7 2,9-Dimethyl-2,3,4,5,6,7-he... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.50	128.75 ng/ul	38477600	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,9-Dimethyl-2,3,4,5,6,7-hexahyd...	203	C14H21N	077581-11-4	53
2	Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	43
3	2,4-Dichlorophenyl isothiocyanate	203	C7H3Cl2NS	006590-96-1	43
4	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	43
5	2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	38





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Quant Title : SVOA CALIBRATION

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

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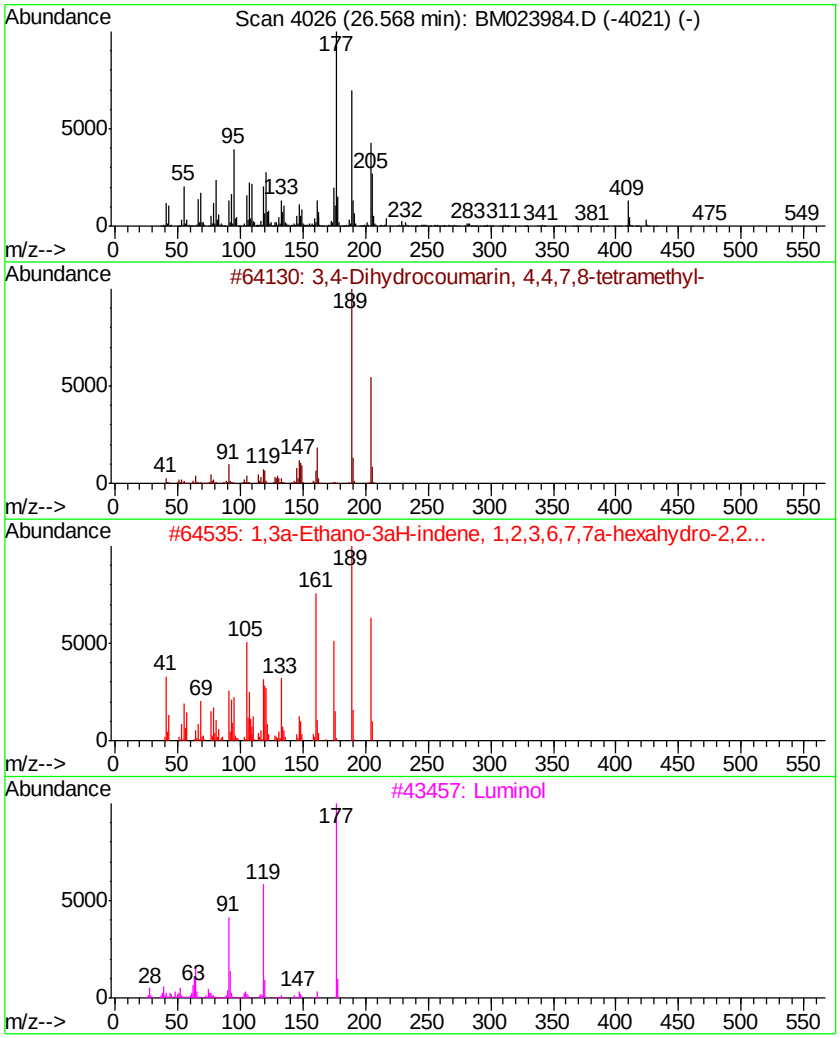
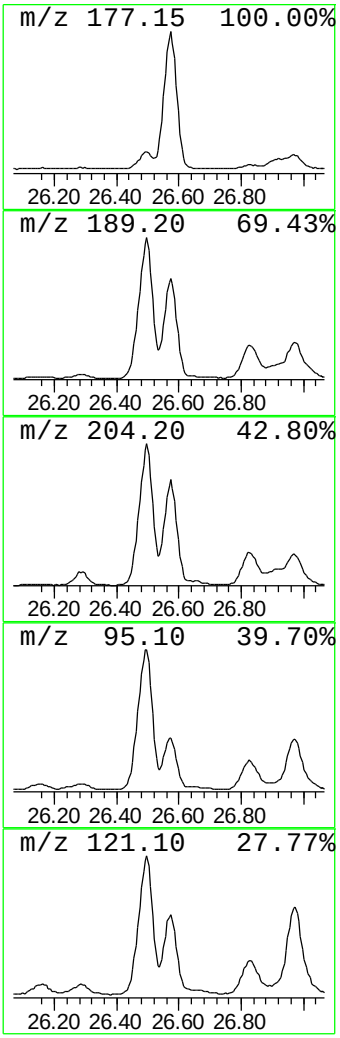
Peak Number 8 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.57	34.66 ng/ul	10359300	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	30
2	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	27
3	Luminol	177	C8H7N3O2	000521-31-3	25
4	Dihydrocoumarin, 4,4,5,7-tetrame...	204	C13H16O2	040662-14-4	25
5	2,10,10-Trimethyltricyclo[7.1.1....	204	C14H20O	1000210-81-9	25





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Data File : BM023984.D
Acq On : 03 Dec 2019 23:49
Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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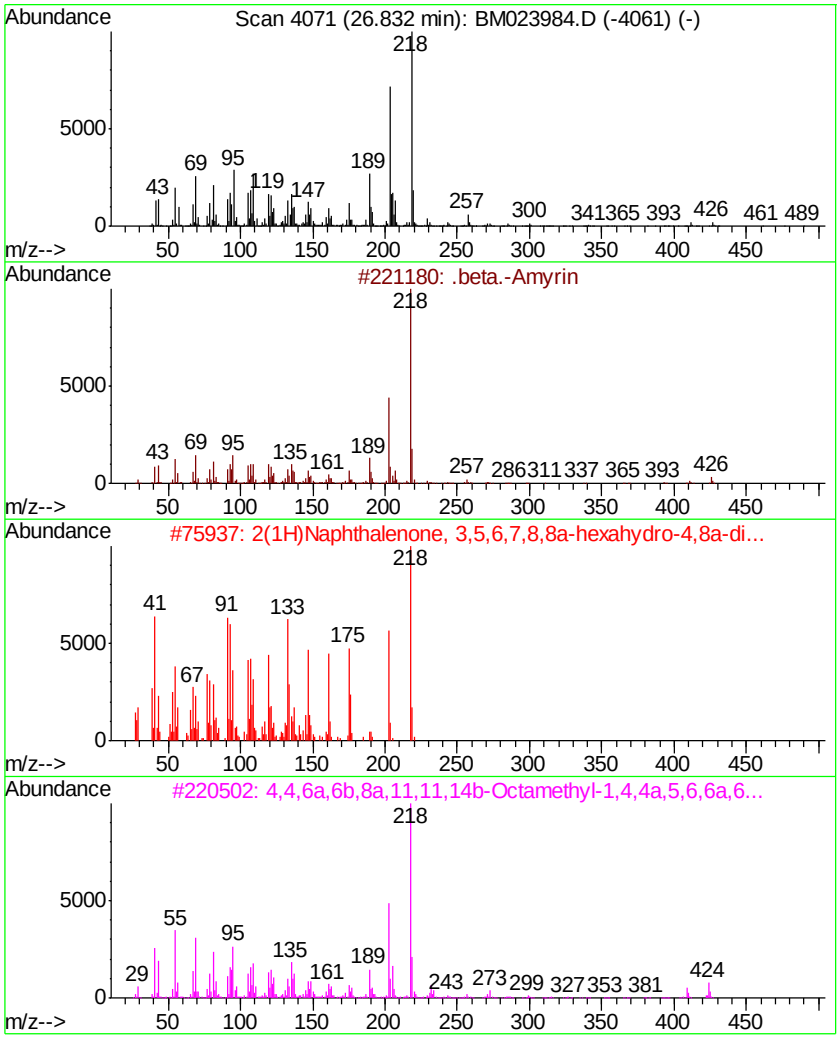
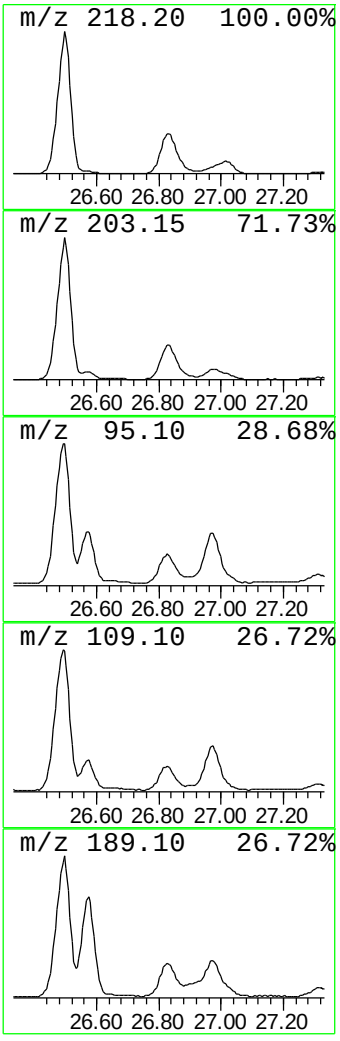
Peak Number 9 .beta.-Amyrin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.83	33.23 ng/ul	9932370	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	87
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	59
3	4,4,6a,6b,8a,11,11,14b-Octamethy...	424	C30H48O	1000194-62-4	58
4	.alpha.-Amyrin	426	C30H50O	000638-95-9	50
5	.beta.-Amyrin	426	C30H50O	000559-70-6	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120319\
Data File : BM023984.D
Acq On : 03 Dec 2019 23:49
Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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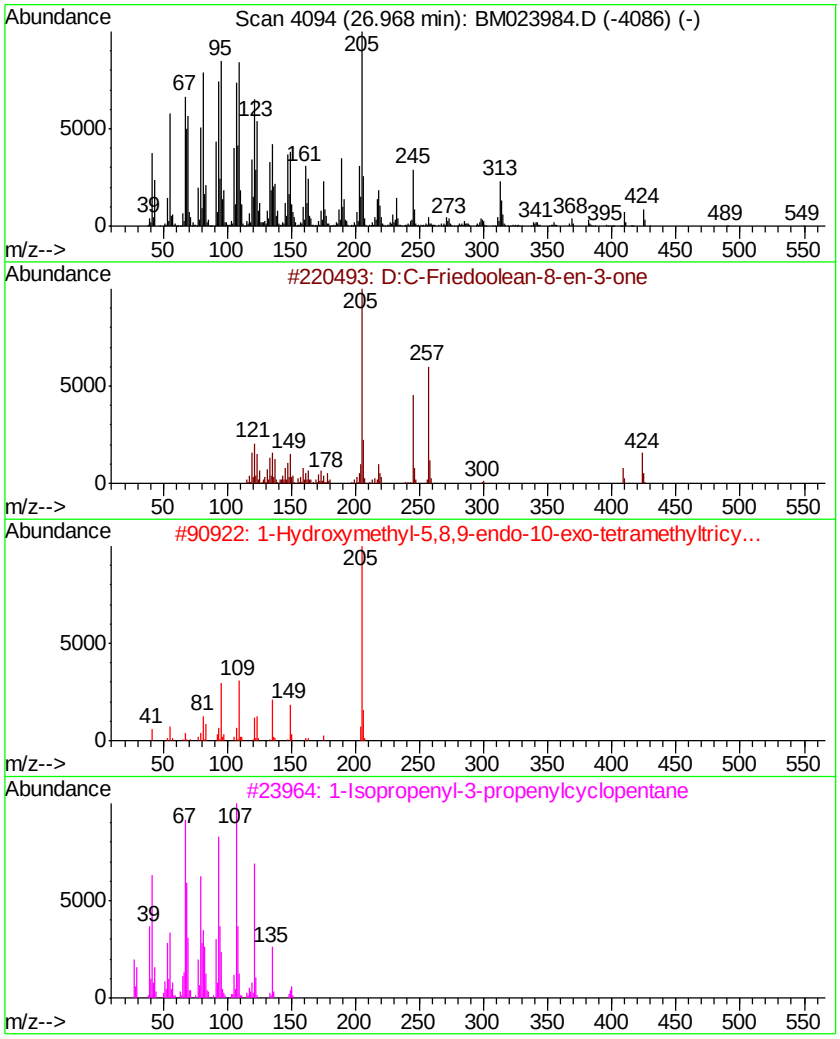
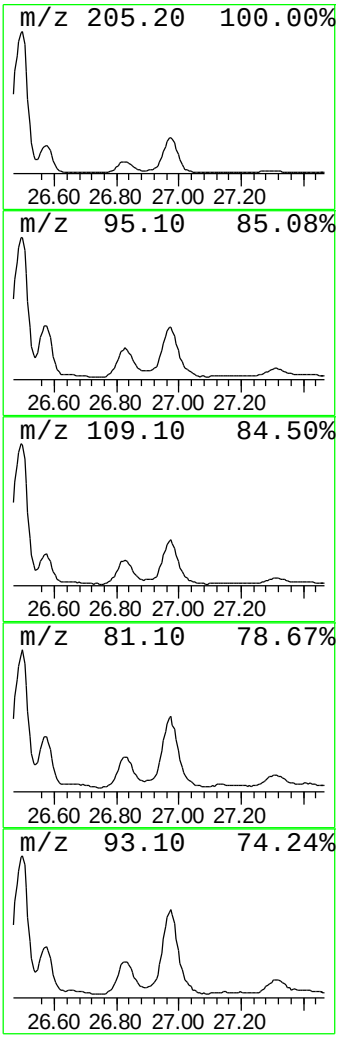
Peak Number 10 D:C-Friedoolean-8-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.97	57.31 ng/ul	17128700	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	91
2	1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	47
3	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	45
4	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	43
5	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	41





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM120319\
Data File : BM023984.D
Acq On : 03 Dec 2019 23:49
Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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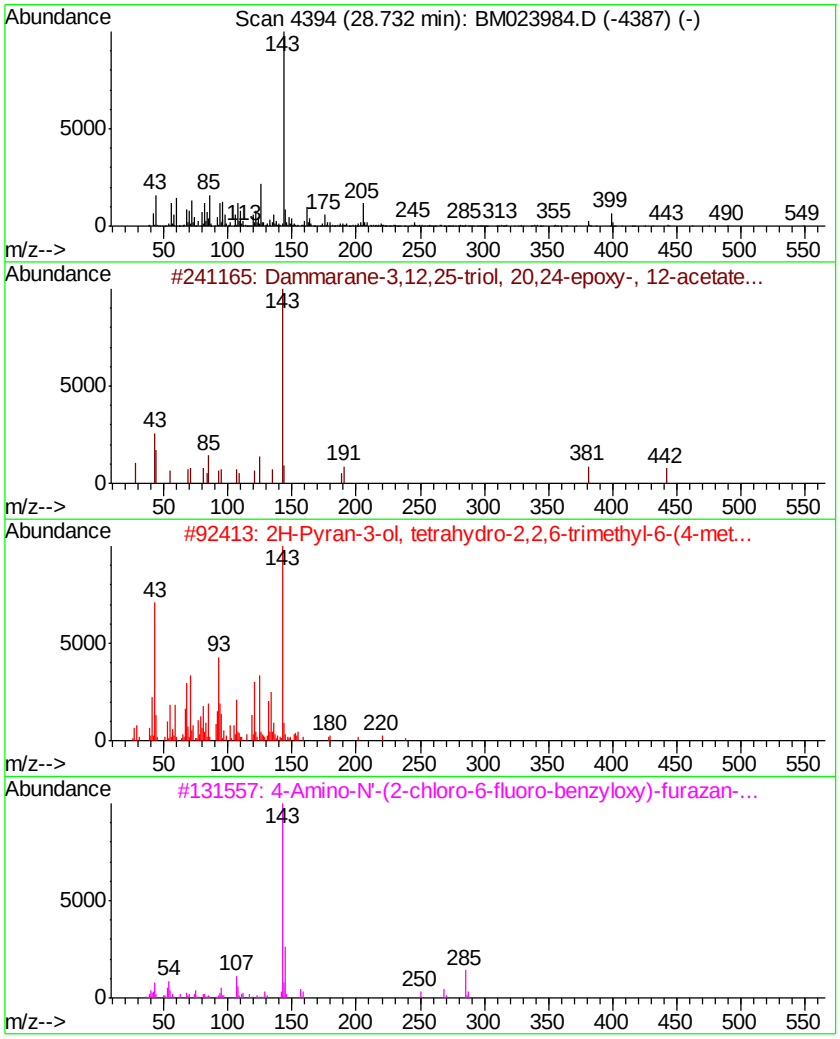
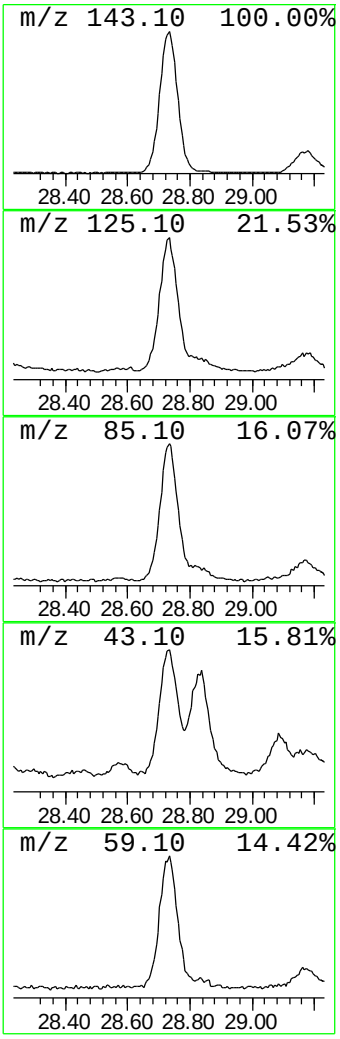
Peak Number 11 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.73	11.03 ng/ul	3297430	Perylene-d12	23.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dammarane-3,12,25-triol, 20,24-e...	604	C35H56O8	078782-15-7	40
2	2H-Pyran-3-ol, tetrahydro-2,2,6-...	238	C15H26O2	022567-36-8	38
3	4-Amino-N'-(2-chloro-6-fluoro-be...	285	C10H9ClFN5O2	1000294-17-1	38
4	p-Fluoro-L-phenylalanine, N-dime...	252	C13H17FN2O2	1000375-82-8	38
5	2-Chloro-6-fluorobenzyl alcohol,...	230	C12H16ClFO	1000378-14-8	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM120319\
Data File : BM023984.D
Acq On : 03 Dec 2019 23:49
Operator : JU
Sample : K5914-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNT0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.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
n-Hexadecanoic acid	17.82	2.1	ng/ul	379182	4	16.90	3572870	20.0
Sulfurous acid, p...	20.84	5.5	ng/ul	1205130	5	21.10	4409420	20.0
(DEL) Alkane: Str...	21.70	11.0	ng/ul	2431370	5	21.10	4409420	20.0
(DEL) Alkane: Cyc...	22.19	4.0	ng/ul	1201480	6	23.24	5977240	20.0
(DEL) Alkane: Str...	22.63	2.5	ng/ul	739851	6	23.24	5977240	20.0
unknown-01	23.53	2.5	ng/ul	748331	6	23.24	5977240	20.0
2,9-Dimethyl-2,3,...	26.50	128.8	ng/ul	38477600	6	23.24	5977240	20.0
unknown-02	26.57	34.7	ng/ul	10359300	6	23.24	5977240	20.0
.beta.-Amyrin	26.83	33.2	ng/ul	9932370	6	23.24	5977240	20.0
D:C-Friedoolean-8...	26.97	57.3	ng/ul	17128700	6	23.24	5977240	20.0
unknown-03	28.73	11.0	ng/ul	3297430	6	23.24	5977240	20.0