LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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	5.563	417	421	429	rVB3	37393	57843	1.31%	0.130%
2	7.075	672	678	691	rBV	310290	550988	12.50%	1.240%
3	7.228	699	704	712	rBV	194548	310785	7.05%	0.699%
4	7.428	732	738	748	rVB	352976	588710	13.35%	1.325%
5	7.887	810	816	825	rVB	507019	807378	18.31%	1.817%
6	8.610	932	939	947	rBV2	404831	660701	14.98%	1.487%
7	9.075	1012	1018	1027	rBV2	294751	461123	10.46%	1.038%
8	9.787	1132	1139	1147	rBV	277198	467929	10.61%	1.053%
9	10.316	1221	1229	1240	rBV	503645	896449	20.33%	2.017%
10	10.692	1285	1293	1300	rBV	588350	1002666	22.74%	2.256%
11	10.857	1315	1321	1330	rBV	338819	618663	14.03%	1.392%
12	13.757	1810	1814	1818	rVB7	34057	47173	1.07%	0.106%
13	13.939	1838	1845	1849	rBV	1073140	1435835	32.56%	3.231%
14	13.986	1849	1853	1859	rVB	452990	619726	14.06%	1.395%
15	14.222	1887	1893	1902	rBV	993120	1487616	33.74%	3.348%
16	14.451	1928	1932	1938	rBV3	41315	63463	1.44%	0.143%
17	14.527	1938	1945	1953	rVB2	993976	1464046	33.20%	3.295%
18	14.769	1981	1986	1992	rVV2	252021	431325	9.78%	0.971%
19	15.516	2106	2113	2120	rBV	1481281	2104699	47.73%	4.736%
20	15.645	2129	2135	2141	rBV2	383797	566943	12.86%	1.276%
21	16.169	2220	2224	2228	rBV7	41790	59197	1.34%	0.133%
22	16.245	2233	2237	2243	rVB2	159375	243947	5.53%	0.549%
23	16.498	2276	2280	2284	rBV6	34933	44465	1.01%	0.100%
24	16.633	2300	2303	2307	rBV5	30105	44332	1.01%	0.100%
25	16.716	2313	2317	2322	rBV7	42206	61171	1.39%	0.138%
26	16.810	2329	2333	2341	rBV10	42992	129098	2.93%	0.291%
27	17.274	2405	2412	2421	rVB2	1392544	1977797	44.86%	4.451%
28	17.374	2423	2429	2437	rVB	1706142	2513220	57.00%	5.656%
29	17.539	2453	2457	2461	rVV7	51778	80599	1.83%	0.181%
30	17.863	2508	2512	2520	rBV	97506	178933	4.06%	0.403%
31	18.074	2541	2548	2551	rBV9	55324	119613	2.71%	0.269%
32	18.121	2551	2556	2562	rVV2	392004	550514	12.49%	1.239%
33	18.180	2562	2566	2569	rVB5	78565	118493	2.69%	0.267%
34	18.351	2591	2595	2600	rVB8	29198	45750	1.04%	0.103%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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	18.439	2605	2610	2616	rVV6	147108	318905	7.23%	0.718%
36	18.492	2616	2619	2623	rVB6	67969	79644	1.81%	0.179%
37	18.539	2623	2627	2630	rBV6	55399	87093	1.98%	0.196%
38	18.574	2630	2633	2638	rVB3	67763	106685	2.42%	0.240%
39	18.810	2670	2673	2674	rBV3	73627	74477	1.69%	0.168%
40	19.057	2712	2715	2717	rBV3	76892	76685	1.74%	0.173%
41	19.098	2717	2722	2726	rVV	612929	758614	17.21%	1.707%
42	19.245	2743	2747	2751	rBV7	141314	233833	5.30%	0.526%
43	19.333	2757	2762	2768	rBV3	797014	938991	21.30%	2.113%
44	19.392	2769	2772	2774	rVV4	233488	269140	6.10%	0.606%
45	19.421	2774	2777	2781	rVB3	270887	345433	7.83%	0.777%
46	19.662	2812	2818	2824	rBV	2691124	3614106	81.97%	8.133%
47	20.986	3041	3043	3050	rVB6	144808	189717	4.30%	0.427%
48	21.103	3058	3063	3068	rBV6	387821	794210	18.01%	1.787%
49	21.439	3116	3120	3125	rBV	2554109	3118166	70.72%	7.017%
50	21.956	3206	3208	3212	rVB2	271257	260534	5.91%	0.586%
51	22.945	3373	3376	3383	rVB3	439327	609877	13.83%	1.372%
52	23.627	3486	3492	3499	rVB2	2423757	4409186	100.00%	9.923%
53	23.774	3512	3517	3526	rVB	1695169	3227629	73.20%	7.264%
54	26.868	4036	4043	4049	rBV4	1339714	4111970	93.26%	9.254%

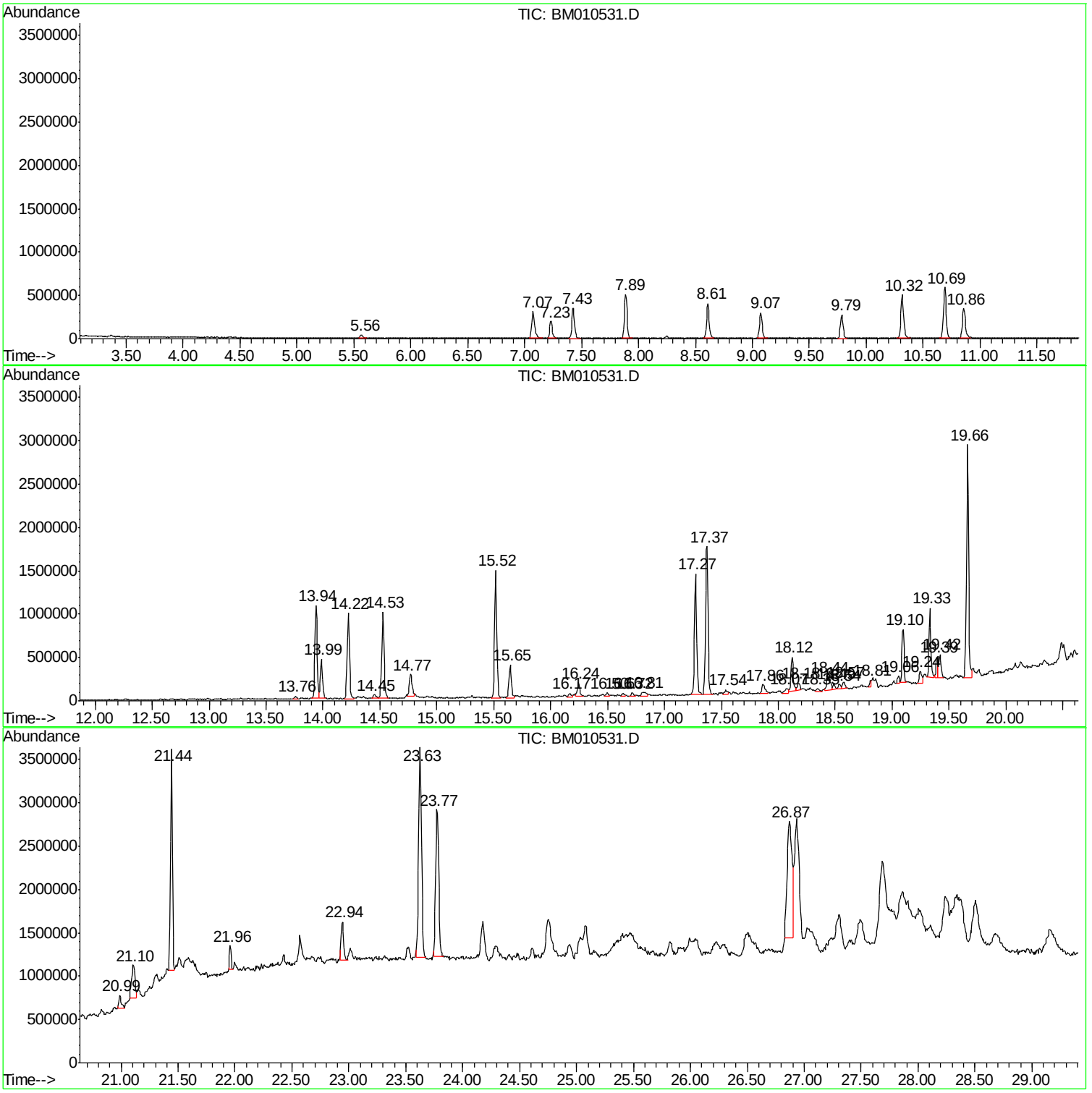
Sum of corrected areas: 44436085

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

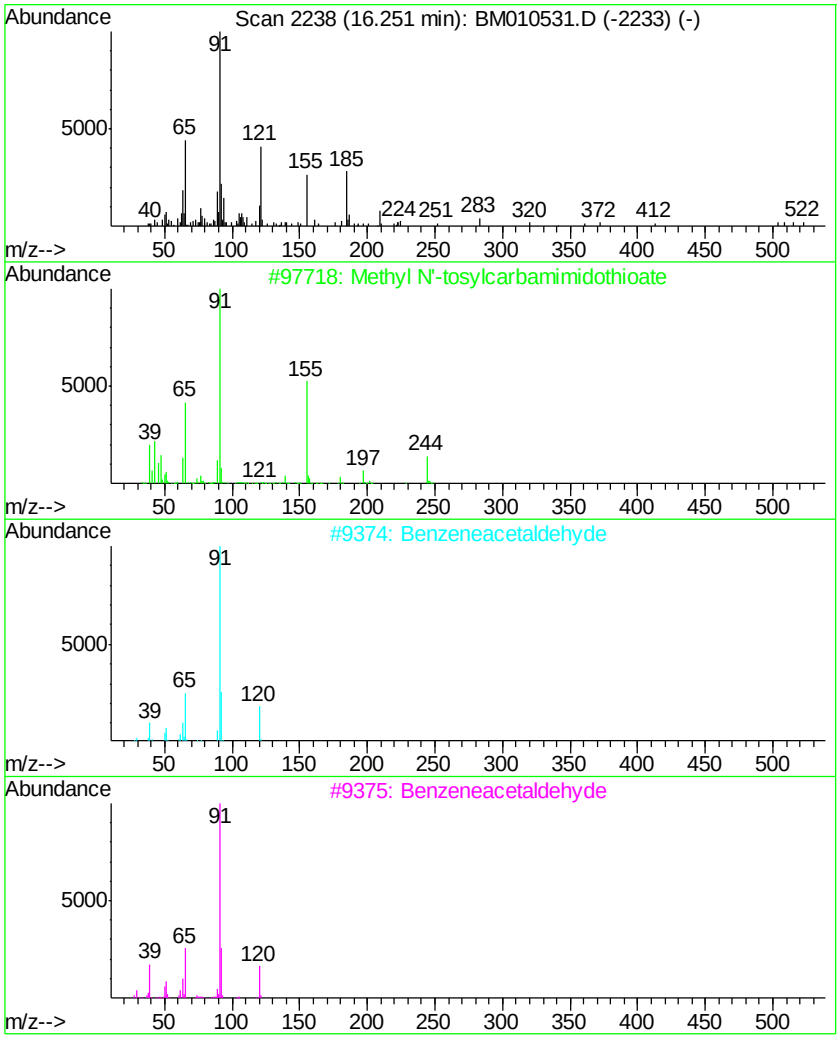
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

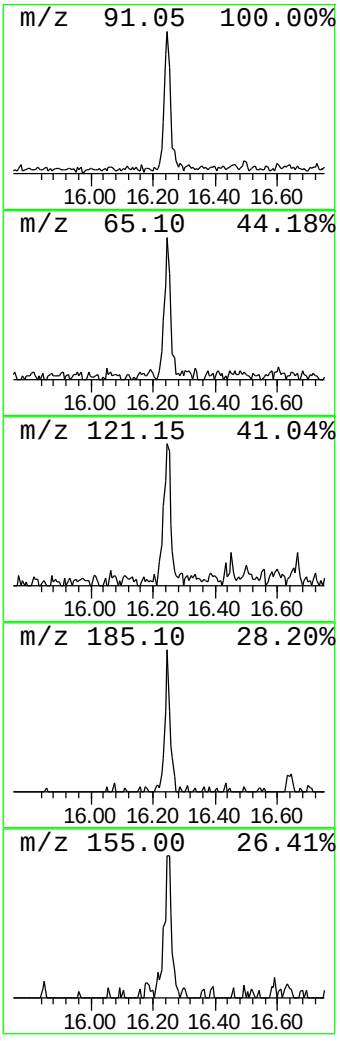
****

Peak Number 1 Methyl N'-tosylcarbamimidot... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.47 ng/ul	243947	Phenanthrene-d10	17.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl N'-tosylcarbamimidothioate	244	C9H12N2O2S2	002651-16-3	59
2	Benzeneacetaldehyde	120	C8H8O	000122-78-1	59
3	Benzeneacetaldehyde	120	C8H8O	000122-78-1	59
4	N-Sulfinyl-p-toluenesulfonamide	217	C7H7NO3S2	004104-47-6	59
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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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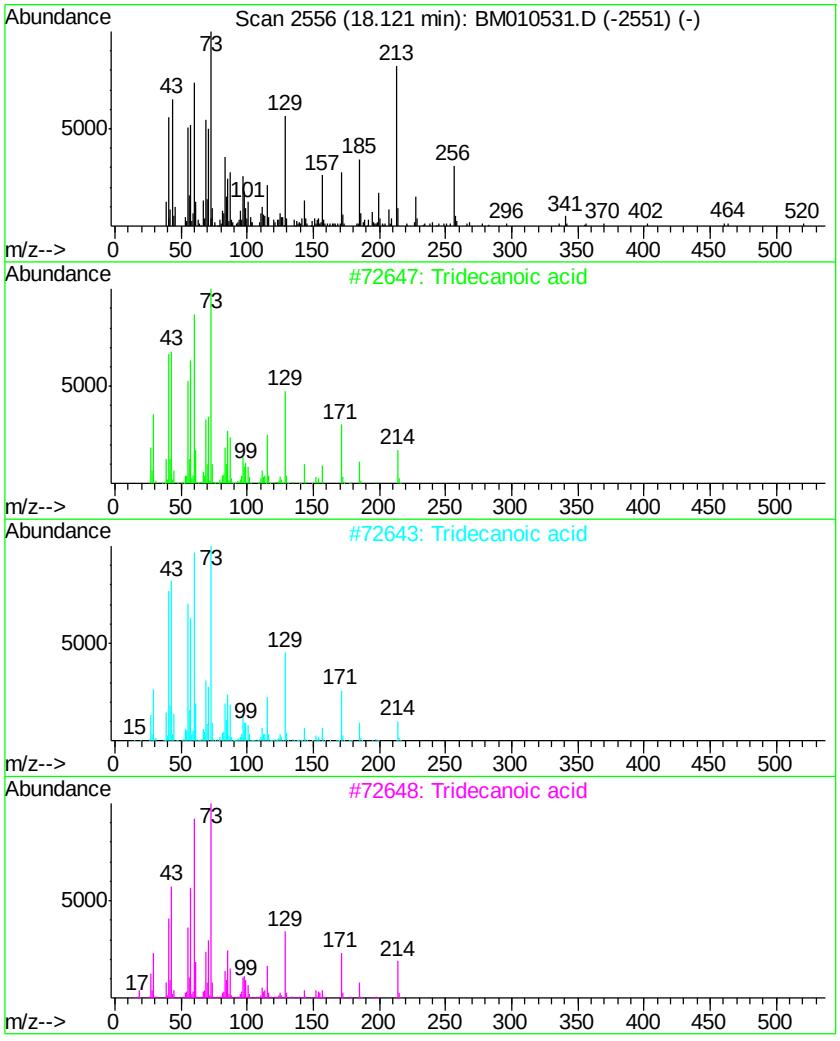
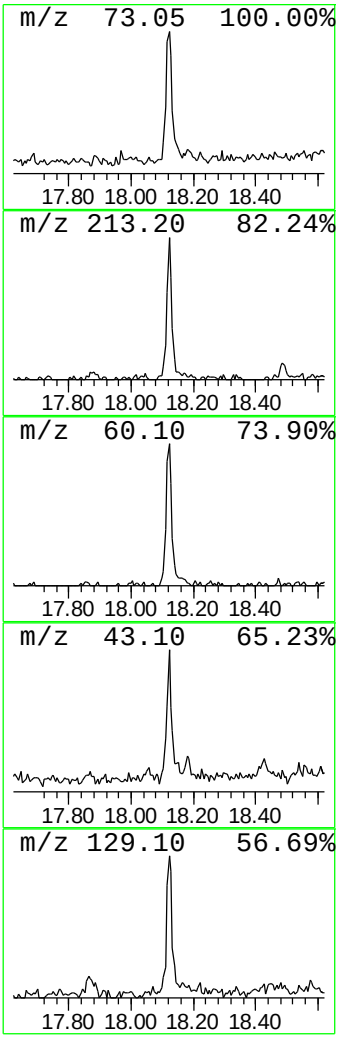
Peak Number 2 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	5.57 ng/ul	550514	Phenanthrene-d10	17.27

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	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	55
4	n-Decanoic acid	172	C10H20O2	000334-48-5	42
5	n-Decanoic acid	172	C10H20O2	000334-48-5	42





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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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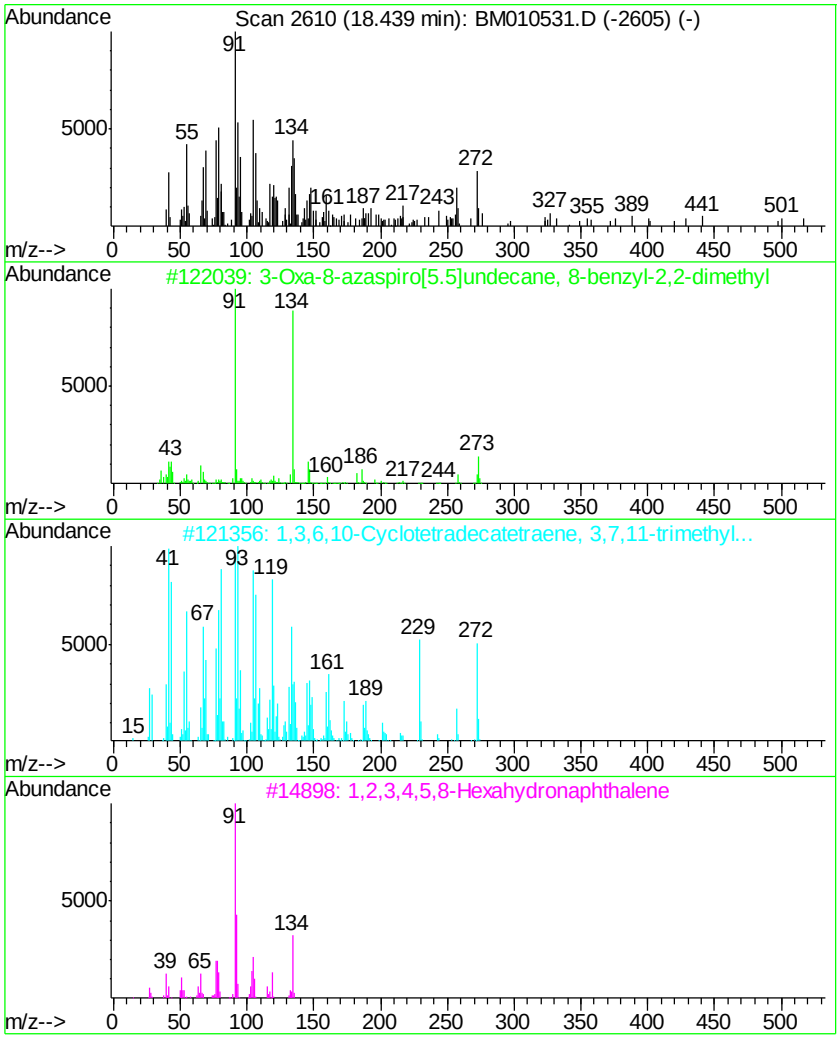
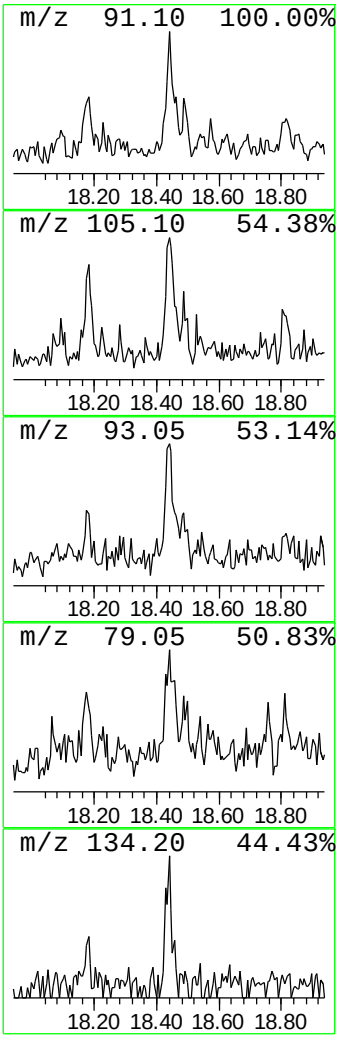
Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	3.22 ng/ul	318905	Phenanthrene-d10	17.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Oxa-8-azaspiro[5.5]undecane, 8...	273	C18H27NO	087399-97-1	32
2	1,3,6,10-Cyclotetradecatetraene,...	272	C20H32	001898-13-1	30
3	1,2,3,4,5,8-Hexahydronaphthalene	134	C10H14	036231-13-7	22
4	Benzene, 2,4-dimethyl-1-nitro-	151	C8H9NO2	000089-87-2	22
5	Benzeneacetaldehyde, 4-methyl-	134	C9H10O	000104-09-6	22





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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

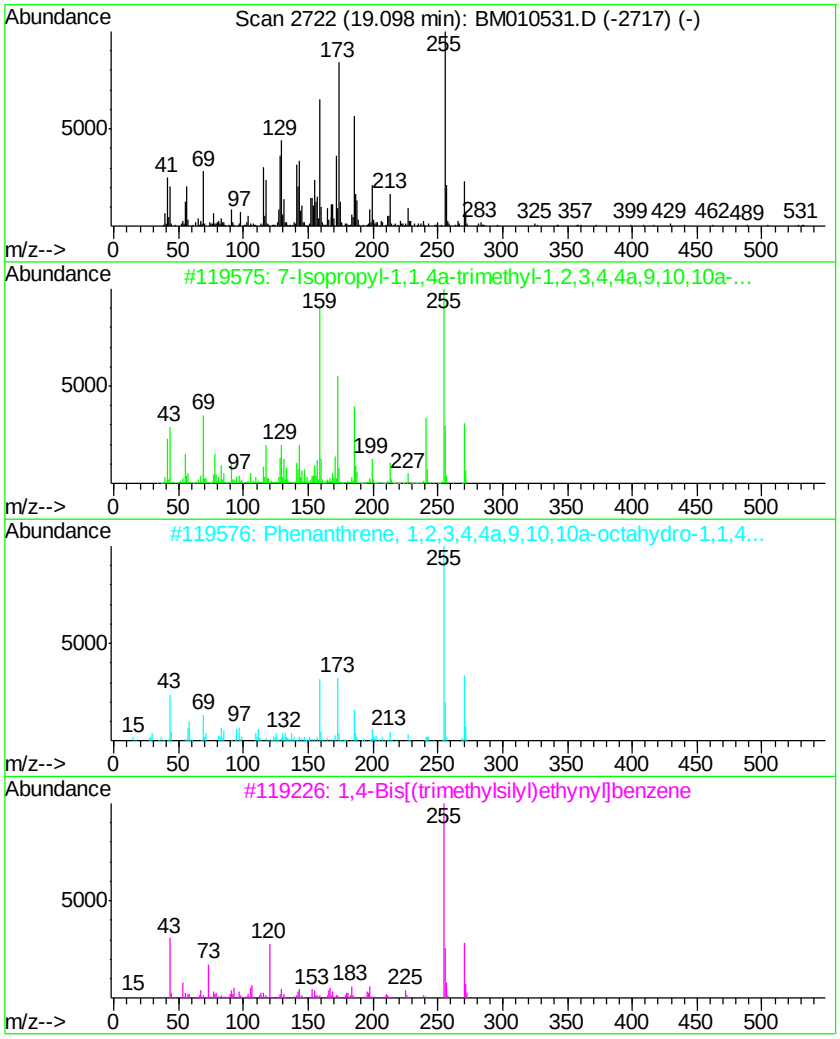
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

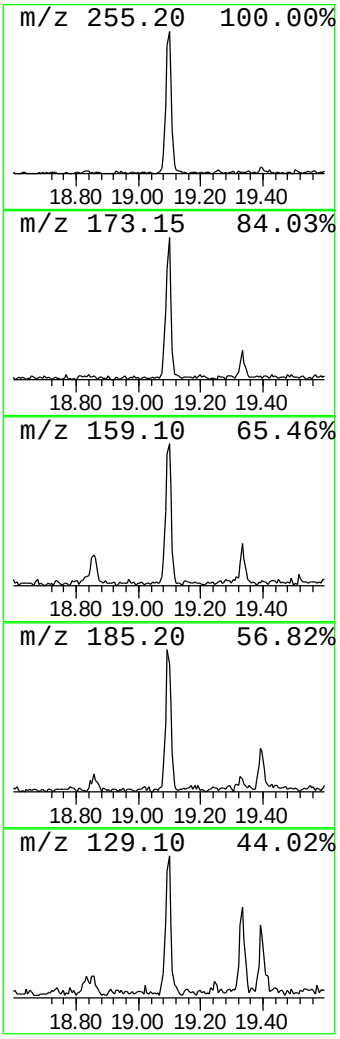
****

Peak Number 4 7-Isopropyl-1,1,4a-trimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.10	7.67 ng/ul	758614	Phenanthrene-d10	17.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Isopropyl-1,1,4a-trimethyl-1,2...	270	C20H30	1000210-28-9	58
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	270	C20H30	019407-28-4	35
3	1,4-Bis[(trimethylsilyl)ethynyl]...	270	C16H22Si2	073392-23-1	25
4	2(5H)-Furanone, 5-(phenylimino)-	173	C10H7NO2	019990-26-2	25
5	Sebacic acid, 3-oxobut-2-yl pent...	342	C19H34O5	1000355-77-6	22





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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

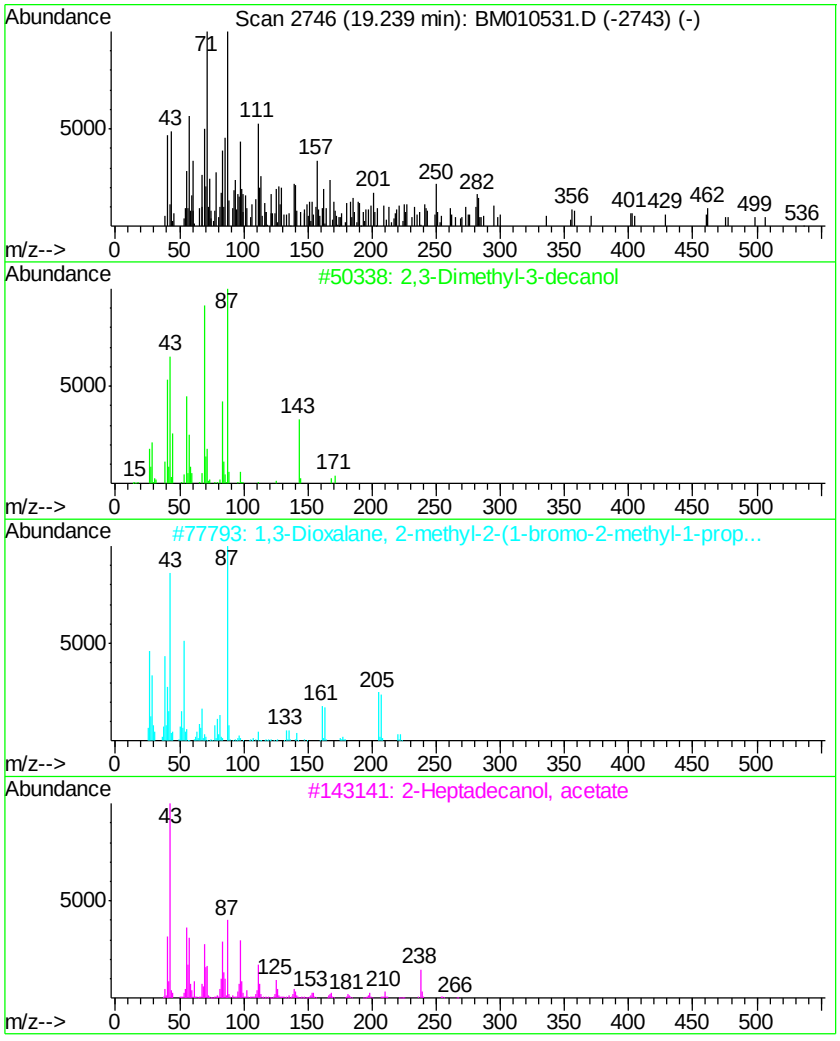
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

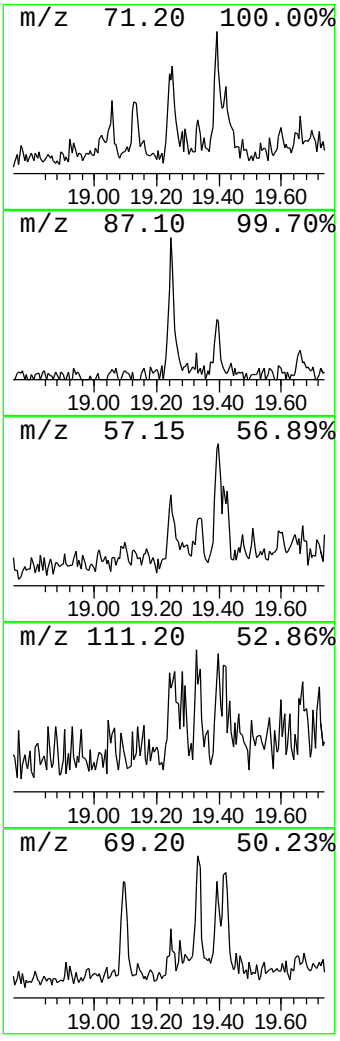
****

Peak Number 5 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	2.36 ng/ul	233833	Phenanthrene-d10	17.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-3-decanol	186	C12H26O	219667-42-2	27
2	1,3-Dioxalane, 2-methyl-2-(1-bro...	220	C8H13BrO2	1000222-00-6	25
3	2-Heptadecanol, acetate	298	C19H38O2	056599-51-0	25
4	2,3,4-Trimethyl-5-hexen-3-ol	142	C9H18O	028638-29-1	22
5	2-Methyl-2-[2-(2,6,6-trimethylcy...	238	C15H26O2	004353-04-2	22





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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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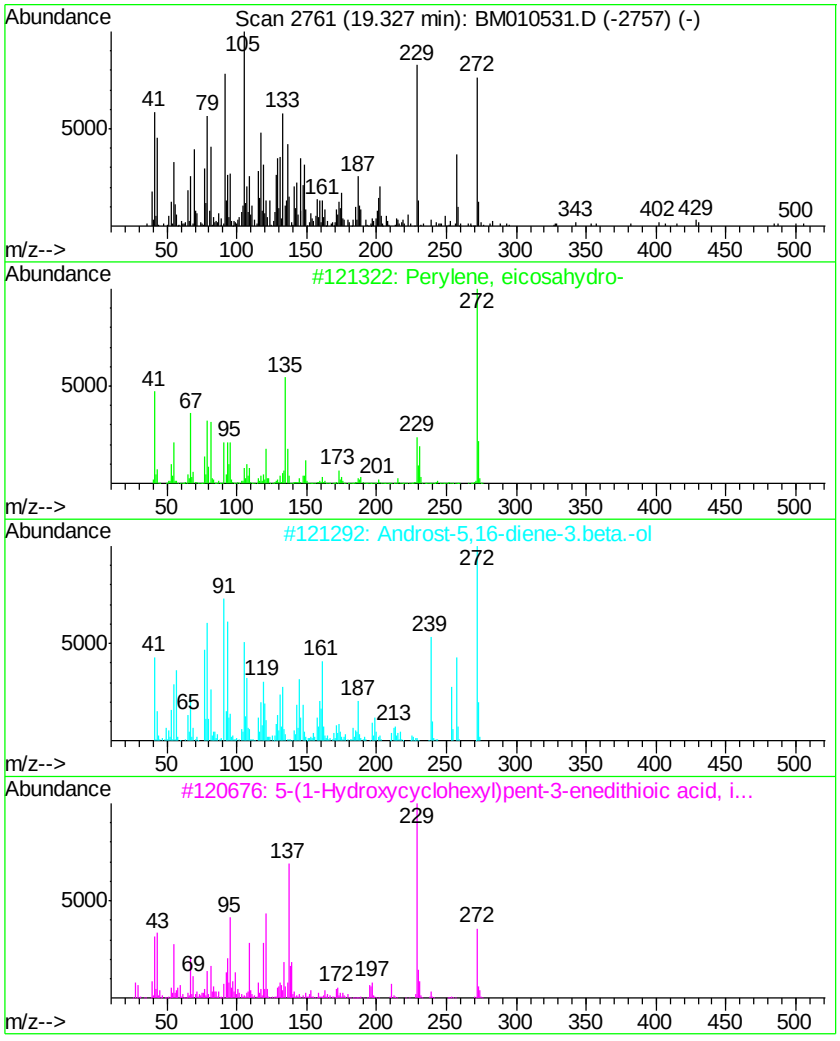
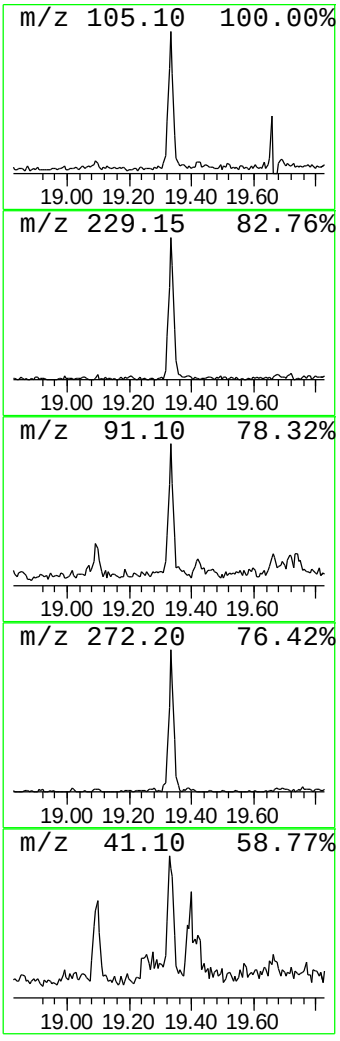
Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	9.50 ng/ul	938991	Phenanthrene-d10	17.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene, eicosahydro-	272	C20H32	047041-72-5	47
2	Androst-5,16-diene-3.beta.-ol	272	C19H28O	001224-94-8	46
3	5-(1-Hydroxycyclohexyl)pent-3-en...	272	C14H24OS2	083041-14-9	46
4	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	020070-61-5	45
5	2,4-Diamino-5-[3,4-isopropyliden...	272	C14H16N4O2	063124-61-8	38





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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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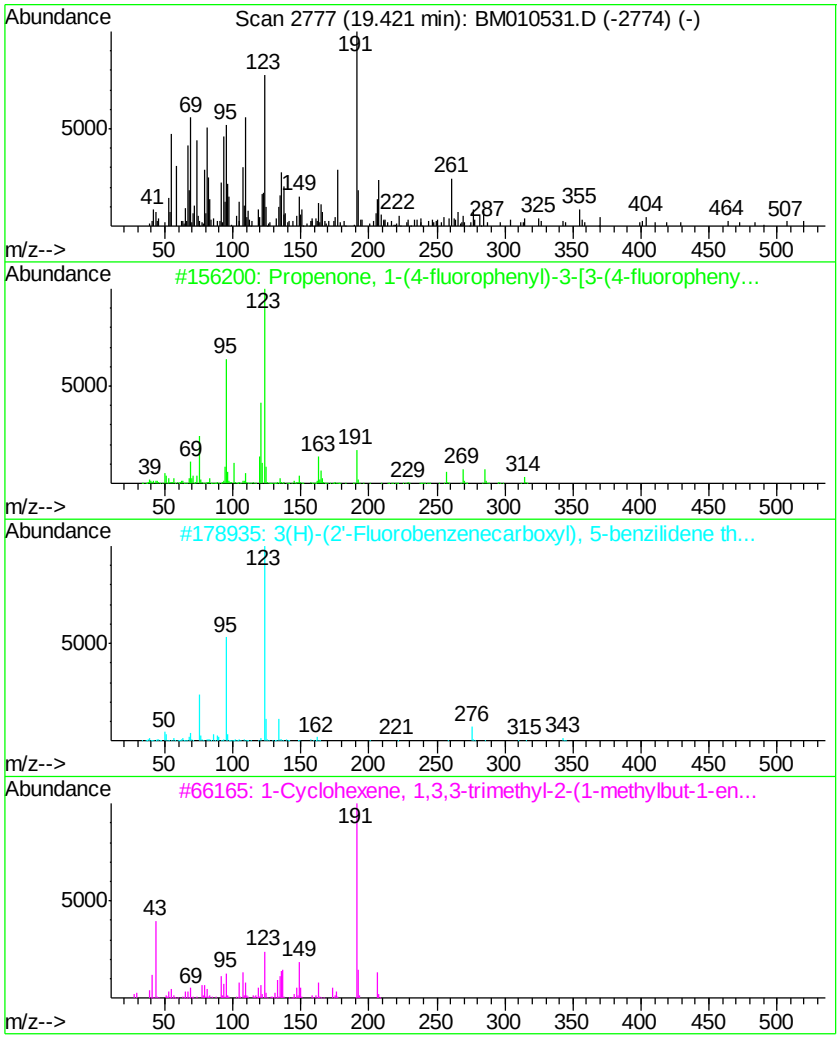
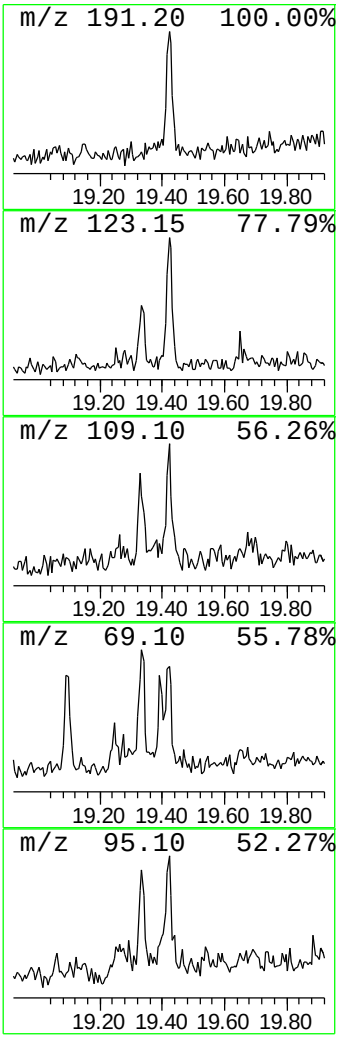
Peak Number 7 unknown-04 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.42	2.22 ng/ul	345433	Chrysene-d12	21.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propenone, 1-(4-fluorophenyl)-3-...	314	C18H12F2O3	024477-72-3	38
2	3(H)-(2'-Fluorobenzenecarboxyl),...	343	C17H10FNO2S2	294193-93-4	38
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	30
5	Pyrazol-3-amine, 1-(4-fluorobenz...	191	C10H10FN3	1000272-83-2	30





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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

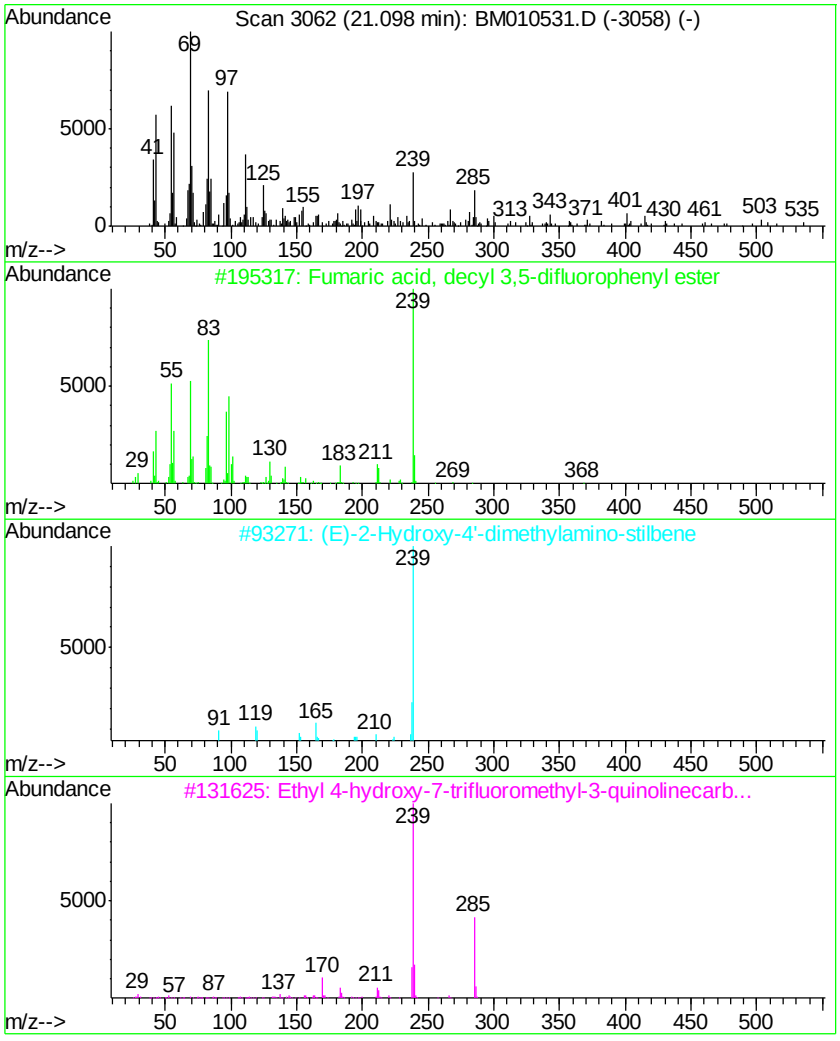
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

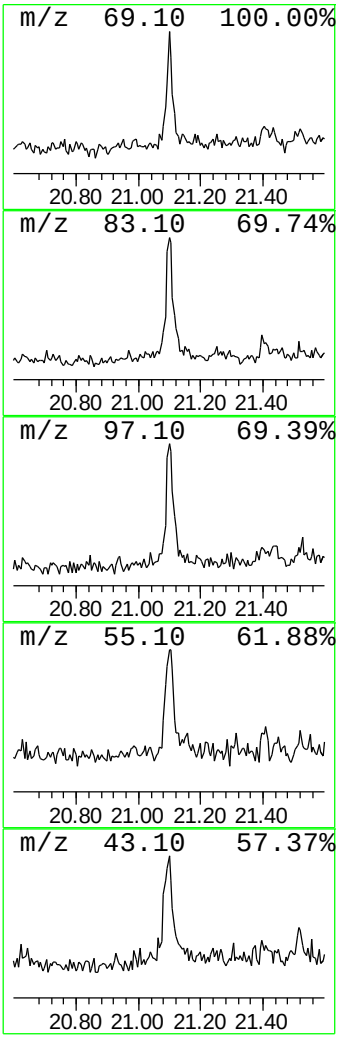
****

Peak Number 8 unknown-05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	5.09 ng/ul	794210	Chrysene-d12	21.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, decyl 3,5-difluoro...	368	C20H26F2O4	1000339-37-6	49
2	(E)-2-Hydroxy-4'-dimethylamino-s...	239	C16H17NO	110983-42-1	38
3	Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3NO3	000391-02-6	30
4	Fumaric acid, 4-cyanophenyl decy...	357	C21H27NO4	1000344-81-8	27
5	Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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

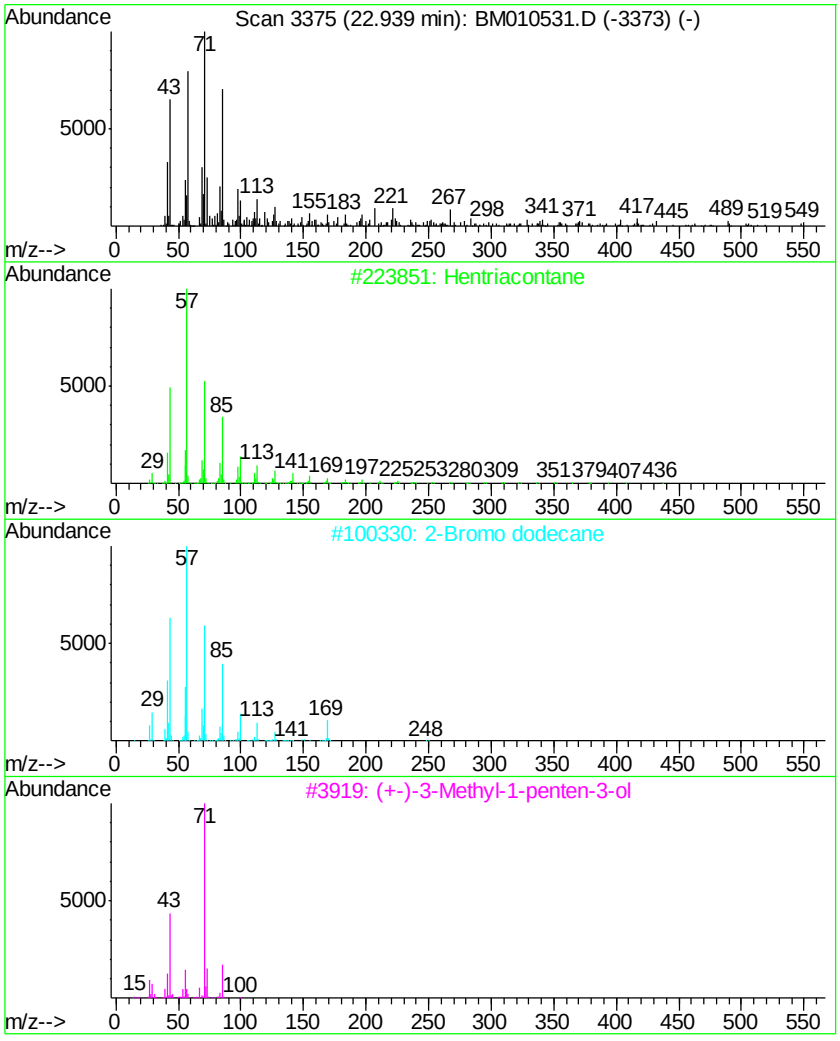
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

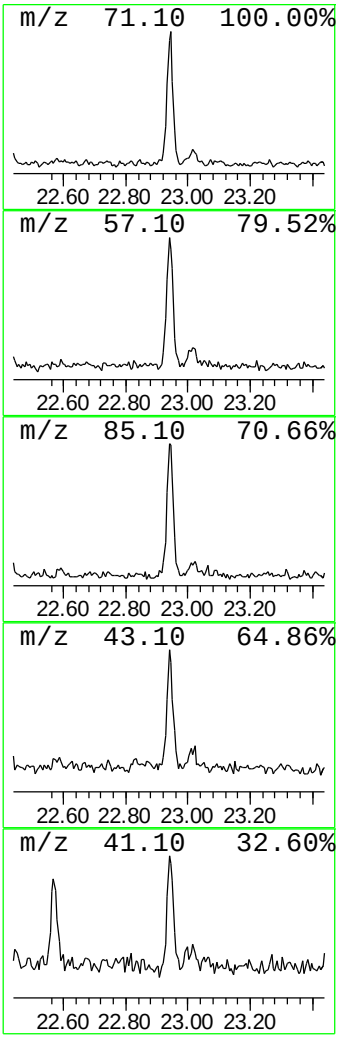
****

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.94	3.78 ng/ul	609877	Perylene-d12	23.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	94
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	87
3	(+-)-3-Methyl-1-penten-3-ol	100	C6H12O	086361-10-6	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Tetratetracontane	619	C44H90	007098-22-8	80





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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

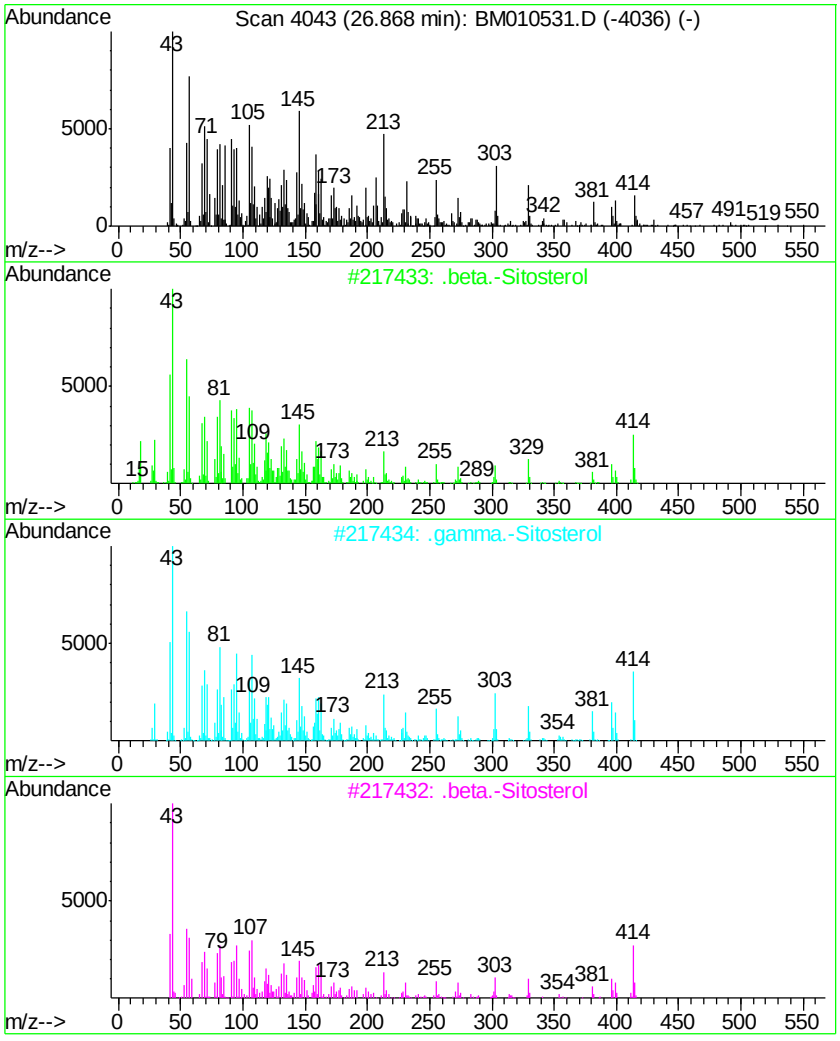
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

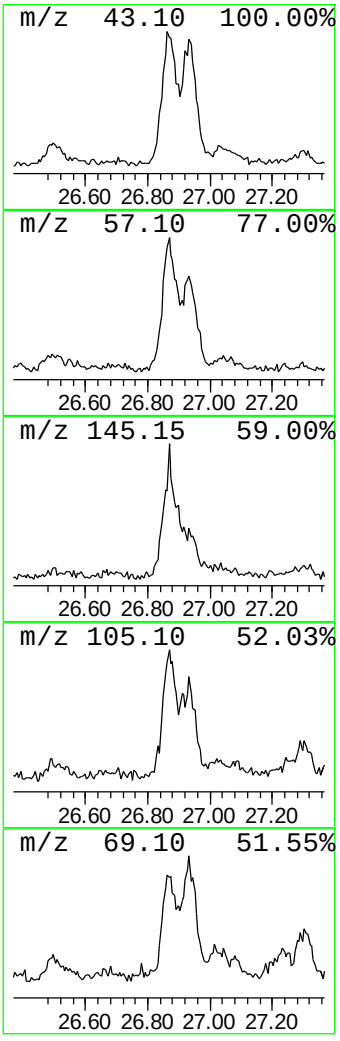
****

Peak Number 10 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.87	25.48 ng/ul	4111970	Perylene-d12	23.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	55
4	Cedran-diol, (8S,14)-	238	C15H26O2	062600-05-9	47
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM061217\
Data File : BM010531.D
Acq On : 12 Jun 2017 12:42
Operator : SJ/MA
Sample : I3571-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : H2TR6

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
Methyl N'-tosylca...	16.25	2.5	ng/ul	243947	4	17.27	1977800	20.0
Tridecanoic acid	18.12	5.6	ng/ul	550514	4	17.27	1977800	20.0
unknown-01	18.44	3.2	ng/ul	318905	4	17.27	1977800	20.0
7-Isopropyl-1,1,4...	19.10	7.7	ng/ul	758614	4	17.27	1977800	20.0
unknown-02	19.24	2.4	ng/ul	233833	4	17.27	1977800	20.0
unknown-03	19.33	9.5	ng/ul	938991	4	17.27	1977800	20.0
unknown-04	19.42	2.2	ng/ul	345433	5	21.44	3118170	20.0
unknown-05	21.10	5.1	ng/ul	794210	5	21.44	3118170	20.0
(DEL) Alkane: Str...	22.94	3.8	ng/ul	609877	6	23.77	3227630	20.0
.beta.-Sitosterol	26.87	25.5	ng/ul	4111970	6	23.77	3227630	20.0