

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
 Data File : BG025731.D
 Acq On : 1 Feb 2017 00:23
 Operator : SJ/MA
 Sample : I1460-20
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BDNR5

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG011817.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	4.447	272	274	275	rBV	7202	5601	0.25%	0.023%
2	5.176	393	398	400	rBV4	6712	8418	0.38%	0.035%
3	5.417	437	439	442	rVB5	5785	6038	0.27%	0.025%
4	5.904	521	522	526	rBV4	6948	5761	0.26%	0.024%
5	5.946	526	529	532	rBV4	5407	8531	0.38%	0.036%
6	6.557	630	633	639	rBV6	4397	10289	0.46%	0.043%
7	7.144	727	733	734	rBV4	3908	5862	0.26%	0.025%
8	7.332	759	765	785	rBV3	187532	489824	21.88%	2.055%
9	7.485	785	791	805	rVB	182599	337986	15.09%	1.418%
10	7.702	821	828	846	rVB	218234	443316	19.80%	1.860%
11	7.861	851	855	857	rVB3	4709	5670	0.25%	0.024%
12	7.967	870	873	875	rVB4	6273	6399	0.29%	0.027%
13	8.172	900	908	924	rBV	243398	504137	22.52%	2.115%
14	8.437	951	953	958	rBV3	4895	6771	0.30%	0.028%
15	8.507	962	965	967	rBV4	4717	5759	0.26%	0.024%
16	8.889	1024	1030	1045	rBV2	232325	515615	23.03%	2.163%
17	9.083	1061	1063	1067	rVB4	8603	5915	0.26%	0.025%
18	9.353	1102	1109	1127	rBV	237223	499813	22.32%	2.097%
19	9.471	1127	1129	1133	rVB4	4638	5544	0.25%	0.023%
20	9.653	1156	1160	1167	rVB8	9082	17902	0.80%	0.075%
21	10.082	1225	1233	1245	rBV2	183591	398120	17.78%	1.670%
22	10.476	1298	1300	1306	rVB4	4177	5509	0.25%	0.023%
23	10.640	1320	1328	1349	rBV2	184658	524761	23.44%	2.202%
24	10.993	1380	1388	1401	rVB	375225	712038	31.80%	2.987%
25	11.163	1409	1417	1429	rBV3	54102	172092	7.69%	0.722%
26	11.439	1461	1464	1470	rBV4	6652	9265	0.41%	0.039%
27	11.521	1474	1478	1480	rBV3	5011	6277	0.28%	0.026%
28	11.586	1487	1489	1492	rVB3	4724	5533	0.25%	0.023%
29	11.645	1492	1499	1503	rBV5	6910	14578	0.65%	0.061%
30	11.698	1503	1508	1509	rVB	5926	7156	0.32%	0.030%
31	11.892	1540	1541	1547	rVB2	4369	5533	0.25%	0.023%
32	12.168	1583	1588	1590	rVB3	5275	9496	0.42%	0.040%
33	12.197	1590	1593	1597	rBV3	6363	8728	0.39%	0.037%
34	12.602	1659	1662	1663	rBV	5972	6018	0.27%	0.025%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
 Data File : BG025731.D
 Acq On : 1 Feb 2017 00:23
 Operator : SJ/MA
 Sample : I1460-20
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BDNR5

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG011817.M
 Title : SVOA CALIBRATION

35	12.726	1679	1683	1686	rBV5	5043	7098	0.32%	0.030%
36	12.790	1692	1694	1703	rVB5	4619	10172	0.45%	0.043%
37	12.873	1703	1708	1711	rBV3	4262	7033	0.31%	0.030%
38	13.284	1777	1778	1784	rBV3	4205	8294	0.37%	0.035%
39	13.572	1825	1827	1832	rBV6	6754	8085	0.36%	0.034%
40	13.731	1849	1854	1858	rVB4	3863	6868	0.31%	0.029%
41	13.836	1869	1872	1878	rBV3	5484	13053	0.58%	0.055%
42	14.195	1926	1933	1937	rBV	553899	854076	38.14%	3.583%
43	14.242	1938	1941	1952	rVB	156097	260223	11.62%	1.092%
44	14.418	1969	1971	1977	rVB4	5283	9968	0.45%	0.042%
45	14.494	1977	1984	1995	rBV	654878	1106315	49.41%	4.641%
46	14.641	2005	2009	2014	rVB5	11398	18945	0.85%	0.079%
47	14.800	2028	2036	2047	rBV	629152	1068134	47.70%	4.481%
48	15.076	2078	2083	2101	rBV4	55206	195496	8.73%	0.820%
49	15.552	2158	2164	2165	rBV4	8043	11134	0.50%	0.047%
50	15.587	2165	2170	2175	rVB3	32719	45376	2.03%	0.190%
51	15.787	2196	2204	2216	rBV	913915	1450723	64.79%	6.086%
52	15.946	2225	2231	2242	rBV5	105100	259773	11.60%	1.090%
53	16.034	2243	2246	2252	rVB7	16466	26961	1.20%	0.113%
54	16.198	2272	2274	2278	rBV5	7539	10080	0.45%	0.042%
55	16.380	2303	2305	2310	rVB6	4941	7200	0.32%	0.030%
56	16.439	2310	2315	2324	rBV2	48458	88142	3.94%	0.370%
57	16.774	2370	2372	2378	rVB5	7007	10649	0.48%	0.045%
58	17.232	2445	2450	2456	rBV2	48125	65590	2.93%	0.275%
59	17.285	2456	2459	2463	rVB6	14832	17482	0.78%	0.073%
60	17.544	2496	2503	2513	rBV2	853646	1356668	60.59%	5.692%
61	17.644	2513	2520	2535	rVB2	1010771	1666724	74.44%	6.992%
62	17.767	2538	2541	2546	rBV5	18960	26676	1.19%	0.112%
63	17.820	2546	2550	2557	rVB3	27979	43893	1.96%	0.184%
64	17.967	2571	2575	2583	rVB4	30654	51362	2.29%	0.215%
65	18.701	2697	2700	2704	rVB6	8490	10840	0.48%	0.045%
66	19.071	2759	2763	2767	rBV3	28038	37074	1.66%	0.156%
67	19.118	2767	2771	2776	rVB	54892	75626	3.38%	0.317%
68	19.565	2844	2847	2853	rVB4	16336	20956	0.94%	0.088%
69	19.923	2900	2908	2922	rBV	1392118	2239087	100.00%	9.394%
70	20.182	2947	2952	2955	rBV	341215	394507	17.62%	1.655%
71	20.217	2955	2958	2966	rVB	760136	806994	36.04%	3.386%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

Integration Parameters: LSCINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG011817.M
Title : SVOA CALIBRATION

72	21.175	3116	3121	3124	rBV	132400	175604	7.84%	0.737%
73	21.210	3124	3127	3136	rVB	284721	343684	15.35%	1.442%
74	21.398	3156	3159	3174	rBV	40426	127564	5.70%	0.535%
75	21.833	3226	3233	3246	rBV	1014816	1837357	82.06%	7.708%
76	22.291	3307	3311	3314	rBV4	62145	99174	4.43%	0.416%
77	22.338	3315	3319	3325	rVB4	118357	175307	7.83%	0.735%
78	23.783	3561	3565	3574	rVB3	99351	193588	8.65%	0.812%
79	24.976	3758	3768	3779	rBV2	695840	1999569	89.30%	8.389%
80	25.211	3798	3808	3830	rVB2	578081	1806617	80.69%	7.579%

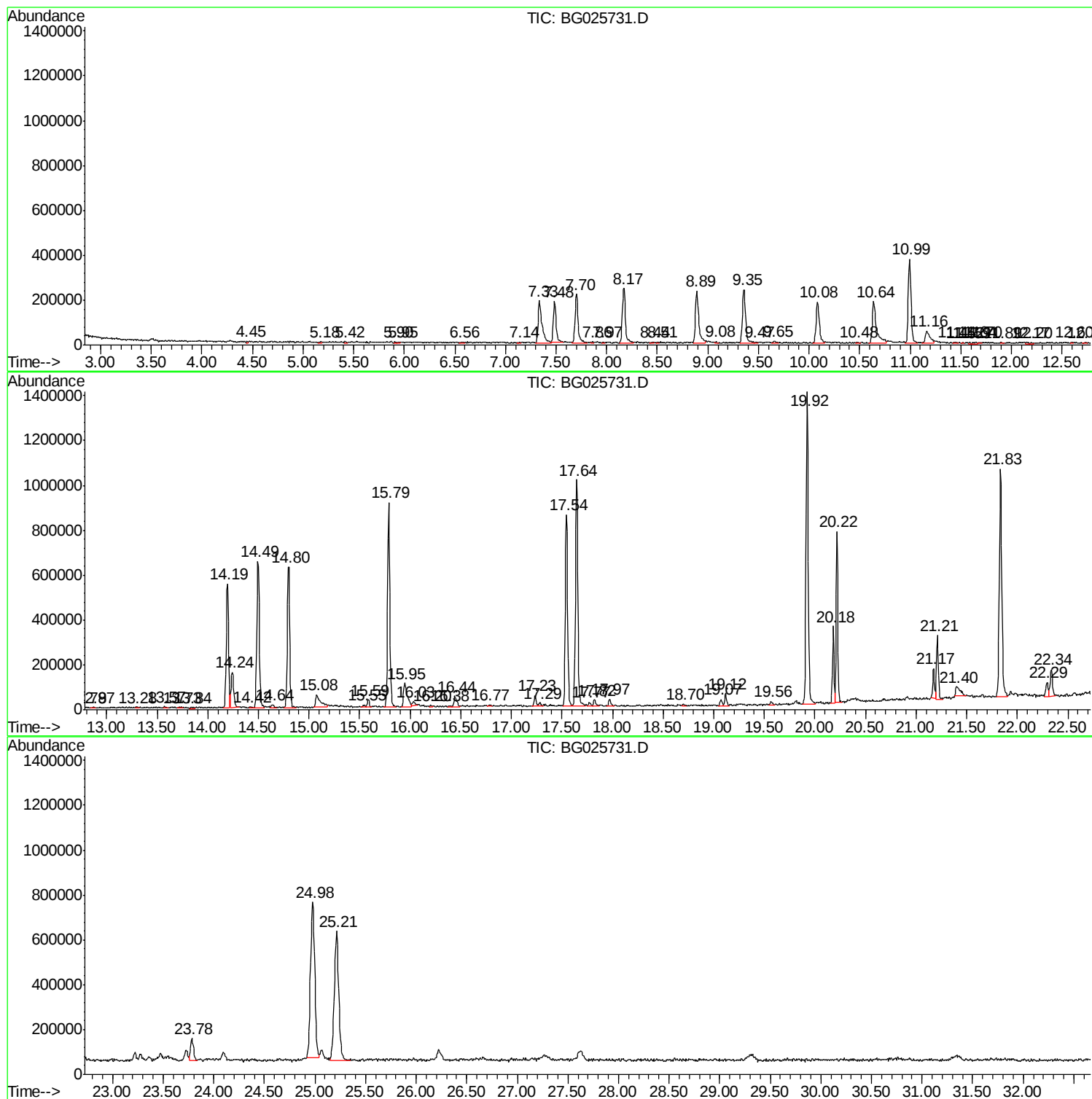
Sum of corrected areas: 23835996

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

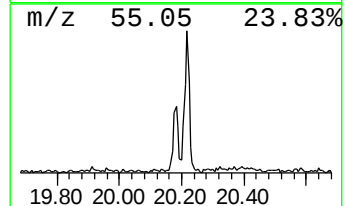
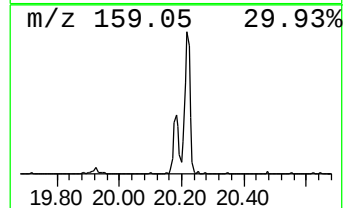
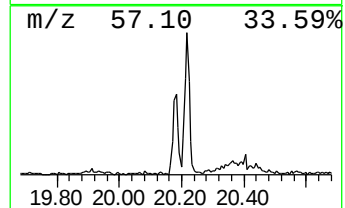
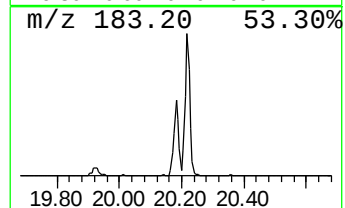
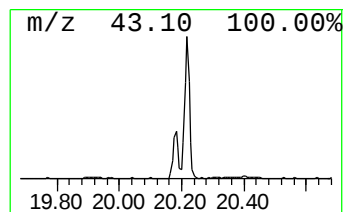
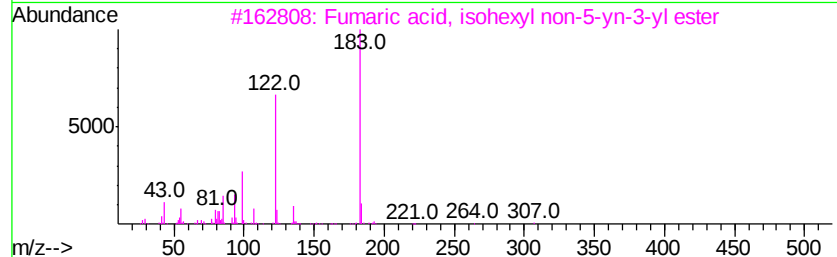
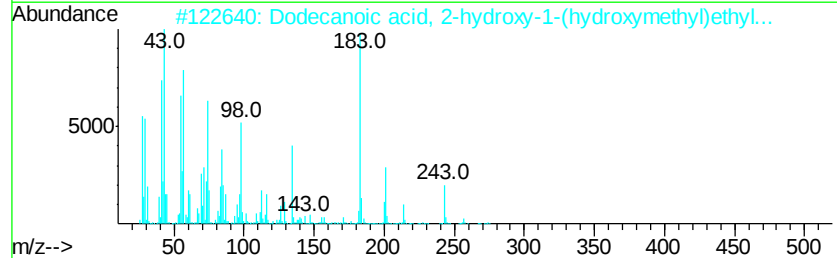
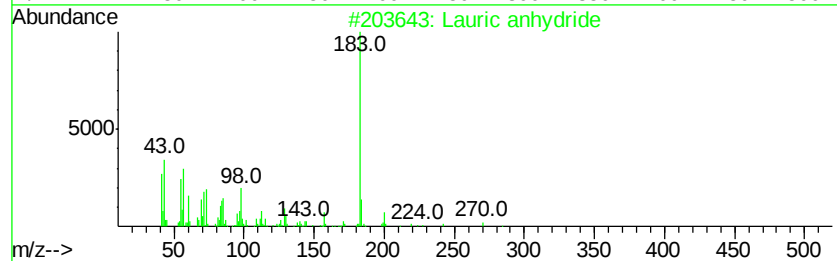
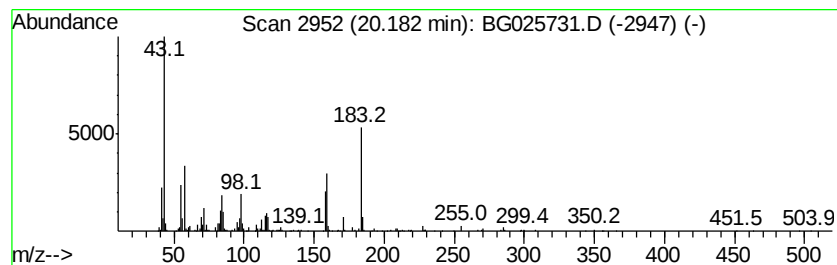
Instrument :
BNA_G
ClientSampleId :
BDNR5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.18	4.29 ng/ul	394507	Chrysene-d12	21.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Lauric anhydride	382 C24H46O3	000645-66-9	38
2	Dodecanoic acid, 2-hydroxy-1-(hy...	274 C15H30O4	001678-45-1	32
3	Fumaric acid, isohexyl non-5-yn-...	322 C19H30O4	1000345-29-3	25
4	Eicosanoic acid, 2-(acetyloxy)-1...	470 C27H50O6	055429-68-0	25
5	Fumaric acid, hexyl 3-hexyl ester	284 C16H28O4	1000348-60-5	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

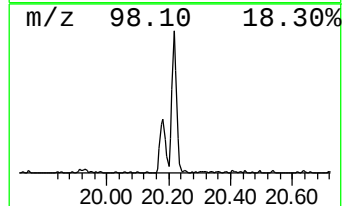
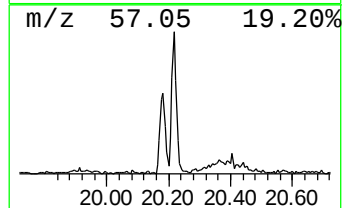
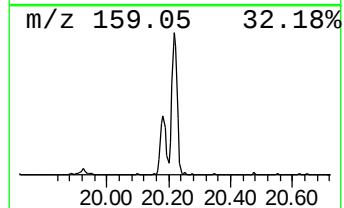
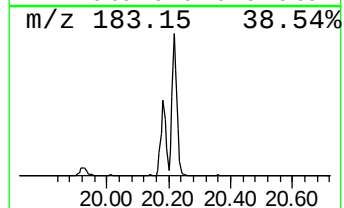
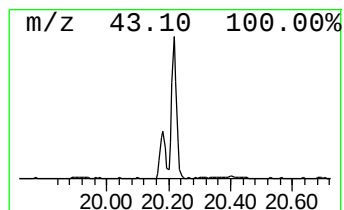
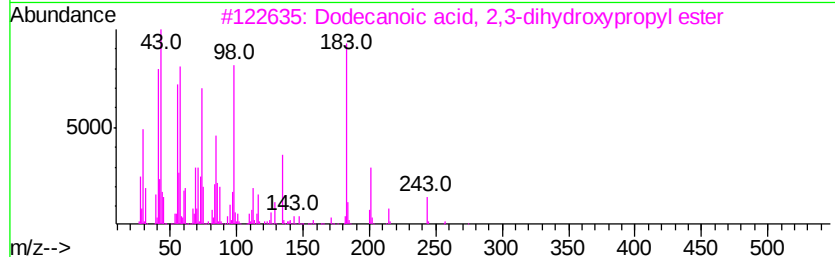
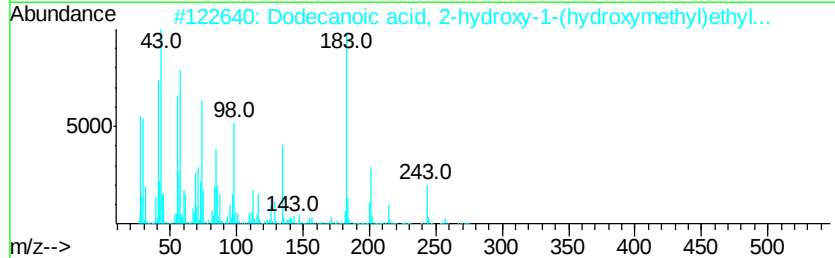
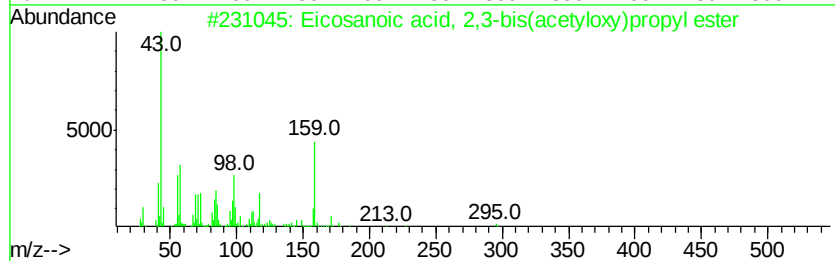
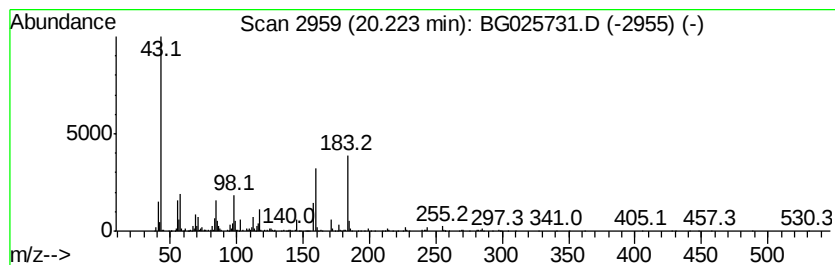
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	8.78 ng/ul	806994	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	40
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	35
3		Dodecanoic acid, 2,3-dihydroxyp...	274	C15H30O4	000142-18-7	25
4		9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	25
5		9-Octadecenoic acid (Z)-, 2-(ace...	440	C25H44O6	055401-63-3	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

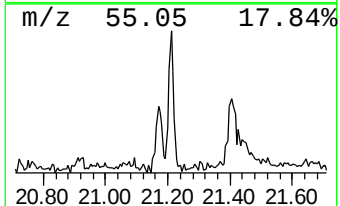
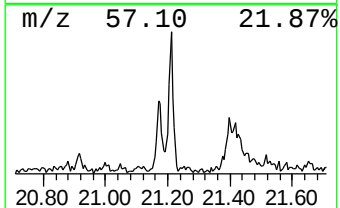
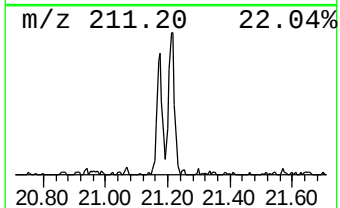
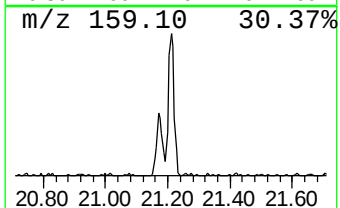
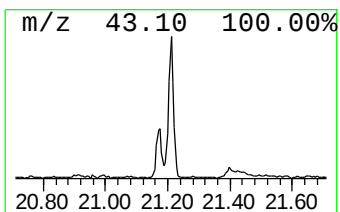
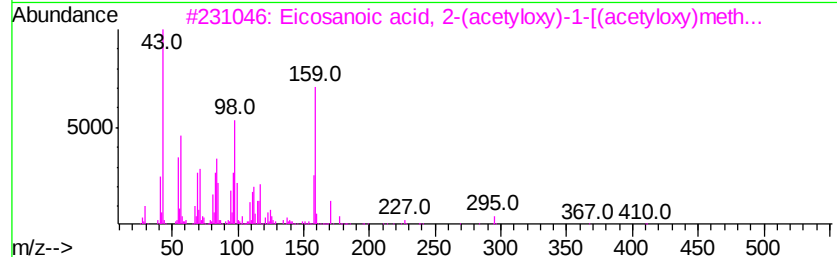
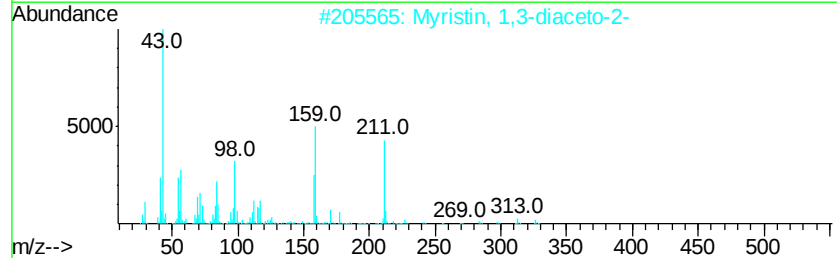
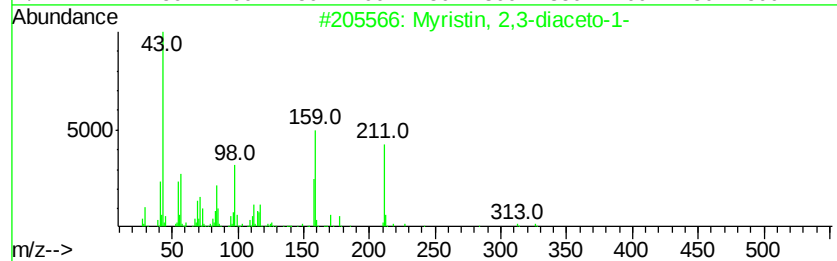
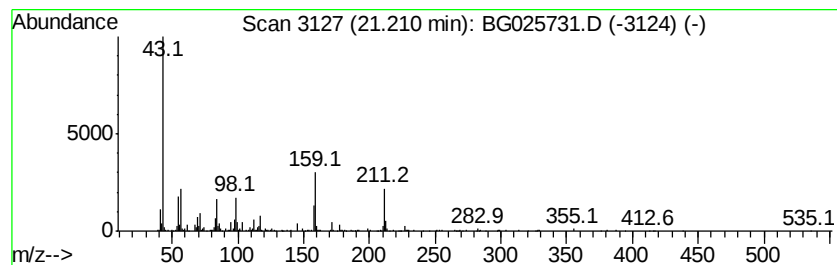
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	3.74 ng/ul	343684	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	80
2		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	72
3		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	14
4		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	12
5		9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

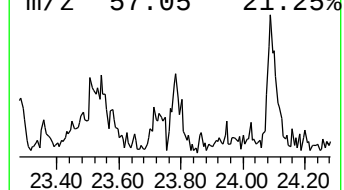
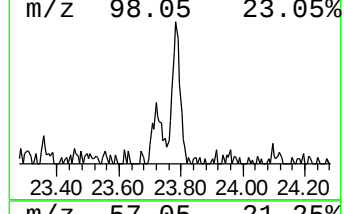
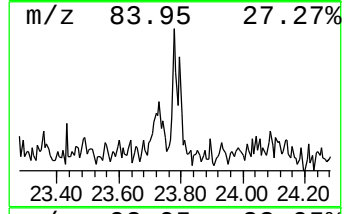
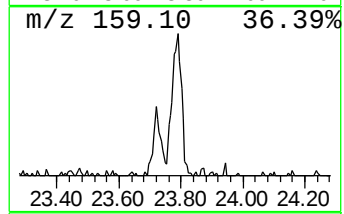
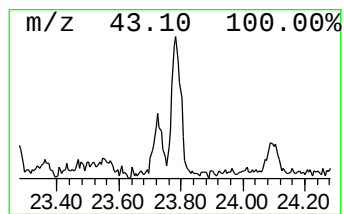
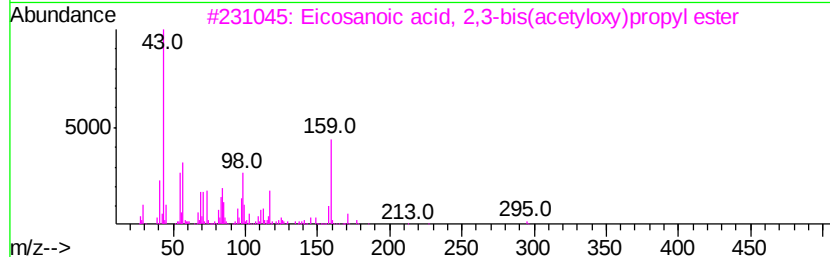
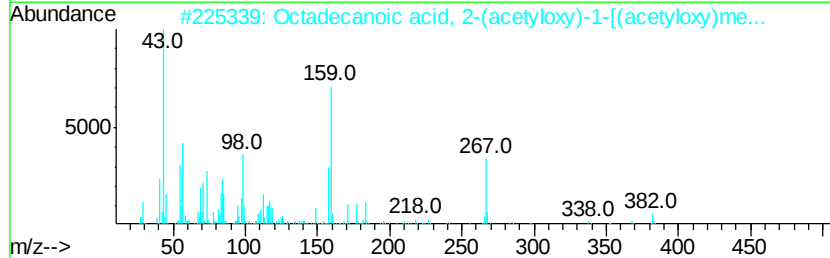
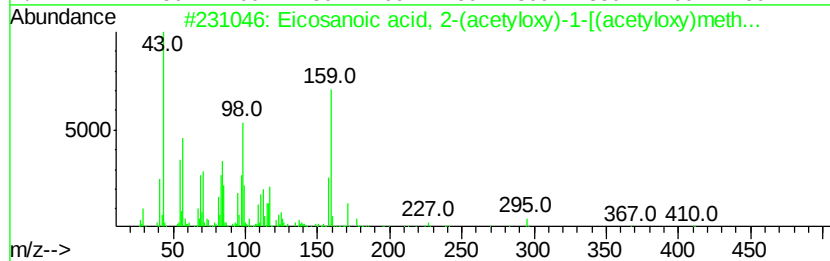
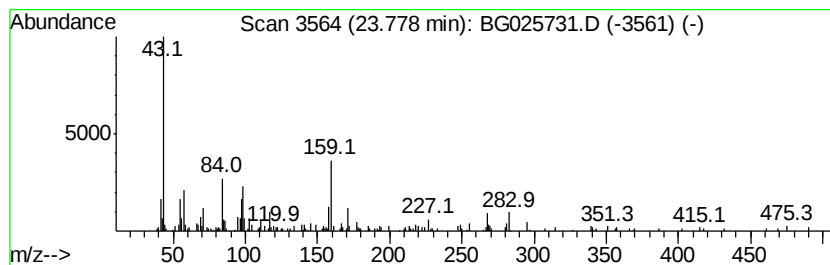
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.78	2.14 ng/ul	193588	Perylene-d12	25.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	25
2		Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	14
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	12
4		9-Methyltricyclo[4.2.1.1(2,5)]de...	178	C11H14O2	078323-73-6	10
5		Thioacetic acid, S-(5-acetylthio...	234	C9H14O3S2	1000185-15-4	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG013117\
Data File : BG025731.D
Acq On : 1 Feb 2017 00:23
Operator : SJ/MA
Sample : I1460-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BDNR5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG011817.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	20.18	4.3	ng/ul	394507	5	21.83	1837360	20.0
unknown-02	20.22	8.8	ng/ul	806994	5	21.83	1837360	20.0
Myristin, 2,3-dia...	21.21	3.7	ng/ul	343684	5	21.83	1837360	20.0
unknown-03	23.78	2.1	ng/ul	193588	6	25.21	1806620	20.0