

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
 Data File : BG026807.D
 Acq On : 1 May 2017 15:18
 Operator : SJ/MA
 Sample : I2850-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JHT81

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\SOM-EPA-BG042717.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	3.429	53	58	64	rBV	19997	30060	1.22%	0.080%
2	4.105	170	173	175	rBV4	3727	5658	0.23%	0.015%
3	4.181	183	186	194	rVB10	3821	7200	0.29%	0.019%
4	4.616	258	260	263	rBV3	6247	5460	0.22%	0.015%
5	4.780	286	288	294	rBV6	3217	5604	0.23%	0.015%
6	4.951	314	317	319	rBV2	6140	6026	0.24%	0.016%
7	6.702	611	615	620	rVB5	4872	8423	0.34%	0.022%
8	7.189	690	698	716	rBV	309536	628035	25.52%	1.671%
9	7.330	716	722	735	rVB	290232	478511	19.44%	1.273%
10	7.548	751	759	777	rBV	346302	632076	25.68%	1.682%
11	7.830	797	807	809	rBV6	4095	9733	0.40%	0.026%
12	8.006	828	837	853	rVV	485710	869055	35.31%	2.313%
13	8.623	940	942	948	rVB4	4210	7663	0.31%	0.020%
14	8.723	953	959	976	rBV	415114	867906	35.27%	2.310%
15	9.087	1019	1021	1025	rVB	4582	6939	0.28%	0.018%
16	9.169	1027	1035	1047	rBV	329984	616207	25.04%	1.640%
17	9.322	1058	1061	1067	rBV4	5026	10198	0.41%	0.027%
18	9.592	1103	1107	1111	rVB3	9050	13220	0.54%	0.035%
19	9.892	1149	1158	1168	rBV	275006	525088	21.34%	1.397%
20	10.256	1215	1220	1225	rVB7	4669	8243	0.33%	0.022%
21	10.444	1244	1252	1274	rBV	419651	859899	34.94%	2.289%
22	10.679	1288	1292	1296	rBV4	4823	5782	0.23%	0.015%
23	10.809	1306	1314	1328	rVB	856038	1516924	61.64%	4.037%
24	10.944	1330	1337	1356	rBV	394967	788237	32.03%	2.098%
25	11.490	1426	1430	1434	rVB6	3317	5296	0.22%	0.014%
26	11.543	1434	1439	1443	rBV5	3018	5984	0.24%	0.016%
27	12.289	1560	1566	1575	rVB7	4470	12508	0.51%	0.033%
28	12.395	1578	1584	1593	rVB6	9436	23862	0.97%	0.064%
29	12.606	1616	1620	1623	rVB4	3991	6249	0.25%	0.017%
30	12.630	1623	1624	1632	rBV4	3072	6578	0.27%	0.018%
31	13.223	1719	1725	1732	rBV8	7653	17451	0.71%	0.046%
32	13.893	1834	1839	1847	rVV7	4352	11042	0.45%	0.029%
33	14.022	1854	1861	1866	rVV	884943	1321626	53.70%	3.517%
34	14.069	1866	1869	1877	rVV	137907	198685	8.07%	0.529%

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35	14.316	1899	1911	1924	rBV	1083752	1713838	69.64%	4.561%
36	14.510	1938	1944	1952	rVB3	17024	24891	1.01%	0.066%
37	14.622	1952	1963	1973	rBV2	1267951	2010918	81.71%	5.352%
38	14.851	1996	2002	2024	rBV	143794	444906	18.08%	1.184%
39	15.062	2036	2038	2042	rVB4	5361	6092	0.25%	0.016%
40	15.127	2045	2049	2057	rVB9	7524	14116	0.57%	0.038%
41	15.192	2057	2060	2068	rVB9	5666	9688	0.39%	0.026%
42	15.350	2083	2087	2090	rVB5	4246	6062	0.25%	0.016%
43	15.409	2090	2097	2101	rBV3	10598	23821	0.97%	0.063%
44	15.456	2101	2105	2111	rVV	42494	52847	2.15%	0.141%
45	15.521	2111	2116	2119	rVV6	3919	5812	0.24%	0.015%
46	15.609	2119	2131	2142	rVV	1376439	2099131	85.30%	5.587%
47	15.732	2144	2152	2167	rBV	281080	458149	18.62%	1.219%
48	15.850	2167	2172	2180	rVB6	26873	53279	2.16%	0.142%
49	15.950	2185	2189	2195	rVB7	5704	9501	0.39%	0.025%
50	16.003	2195	2198	2202	rBV6	8611	10221	0.42%	0.027%
51	16.073	2207	2210	2214	rBV3	8040	10364	0.42%	0.028%
52	16.173	2225	2227	2232	rVB6	4173	6119	0.25%	0.016%
53	16.314	2246	2251	2268	rVV	49976	105362	4.28%	0.280%
54	16.496	2278	2282	2289	rVB8	5122	8183	0.33%	0.022%
55	16.567	2290	2294	2301	rVB9	8295	17226	0.70%	0.046%
56	16.661	2301	2310	2313	rBV8	10159	26694	1.08%	0.071%
57	16.766	2323	2328	2334	rVB8	8530	16529	0.67%	0.044%
58	16.819	2334	2337	2343	rVB6	5949	9770	0.40%	0.026%
59	16.878	2343	2347	2351	rBV7	3906	7239	0.29%	0.019%
60	16.925	2351	2355	2359	rVB7	4070	6310	0.26%	0.017%
61	17.101	2380	2385	2389	rVV	34256	42032	1.71%	0.112%
62	17.154	2389	2394	2400	rVB7	16120	26997	1.10%	0.072%
63	17.248	2405	2410	2414	rBV7	5605	10389	0.42%	0.028%
64	17.354	2420	2428	2438	rBV2	1401603	2061136	83.75%	5.485%
65	17.454	2438	2445	2460	rVB2	1383986	2108457	85.68%	5.611%
66	17.630	2473	2475	2482	rVB8	5264	7786	0.32%	0.021%
67	17.753	2491	2496	2503	rVB9	4358	9180	0.37%	0.024%
68	17.842	2506	2511	2525	rBV10	13862	40961	1.66%	0.109%
69	18.012	2536	2540	2547	rVB6	16341	22633	0.92%	0.060%
70	18.118	2553	2558	2564	rBV9	15967	34406	1.40%	0.092%
71	18.159	2564	2565	2570	rVB5	4275	6331	0.26%	0.017%

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72	18.235	2573	2578	2587	rBV2	126146	225227	9.15%	0.599%
73	18.523	2622	2627	2634	rBV9	9970	25835	1.05%	0.069%
74	18.582	2635	2637	2645	rVV9	6709	12569	0.51%	0.033%
75	18.652	2647	2649	2652	rBV4	6241	5955	0.24%	0.016%
76	19.152	2728	2734	2735	rBV6	10421	17649	0.72%	0.047%
77	19.234	2744	2748	2753	rVB8	9992	20100	0.82%	0.053%
78	19.305	2753	2760	2766	rBV8	17693	35503	1.44%	0.094%
79	19.375	2768	2772	2780	rBV4	20953	39107	1.59%	0.104%
80	19.504	2788	2794	2802	rBV3	66232	136337	5.54%	0.363%
81	19.622	2811	2814	2823	rBV7	12851	32579	1.32%	0.087%
82	19.733	2826	2833	2842	rBV2	1557435	2260574	91.86%	6.016%
83	20.174	2905	2908	2918	rVB2	18885	31314	1.27%	0.083%
84	20.679	2987	2994	3007	rVB2	58705	177188	7.20%	0.472%
85	21.243	3087	3090	3097	rVB7	43644	59293	2.41%	0.158%
86	21.602	3144	3151	3159	rBV	1328594	2150919	87.40%	5.724%
87	22.372	3277	3282	3287	rBV	122246	191500	7.78%	0.510%
88	22.542	3304	3311	3325	rVB3	253637	732762	29.78%	1.950%
89	23.006	3381	3390	3418	rBV3	423225	1773522	72.07%	4.720%
90	23.229	3425	3428	3435	rVB5	50424	85631	3.48%	0.228%
91	23.829	3524	3530	3538	rVB	127572	263792	10.72%	0.702%
92	24.545	3642	3652	3664	rBV2	773077	2127127	86.44%	5.661%
93	24.763	3678	3689	3705	rVB	878686	2460948	100.00%	6.550%
94	25.574	3818	3827	3836	rBV	52130	227205	9.23%	0.605%
95	25.844	3866	3873	3885	rVB4	90447	269524	10.95%	0.717%
96	27.172	4090	4099	4113	rVB5	81167	288724	11.73%	0.768%
97	28.758	4361	4369	4379	rVB5	58999	205336	8.34%	0.546%
98	30.127	4592	4602	4617	rVB5	65646	301531	12.25%	0.802%
99	30.474	4648	4661	4679	rVB6	198995	991010	40.27%	2.637%
100	31.408	4806	4820	4842	rVB6	265259	1376919	55.95%	3.665%

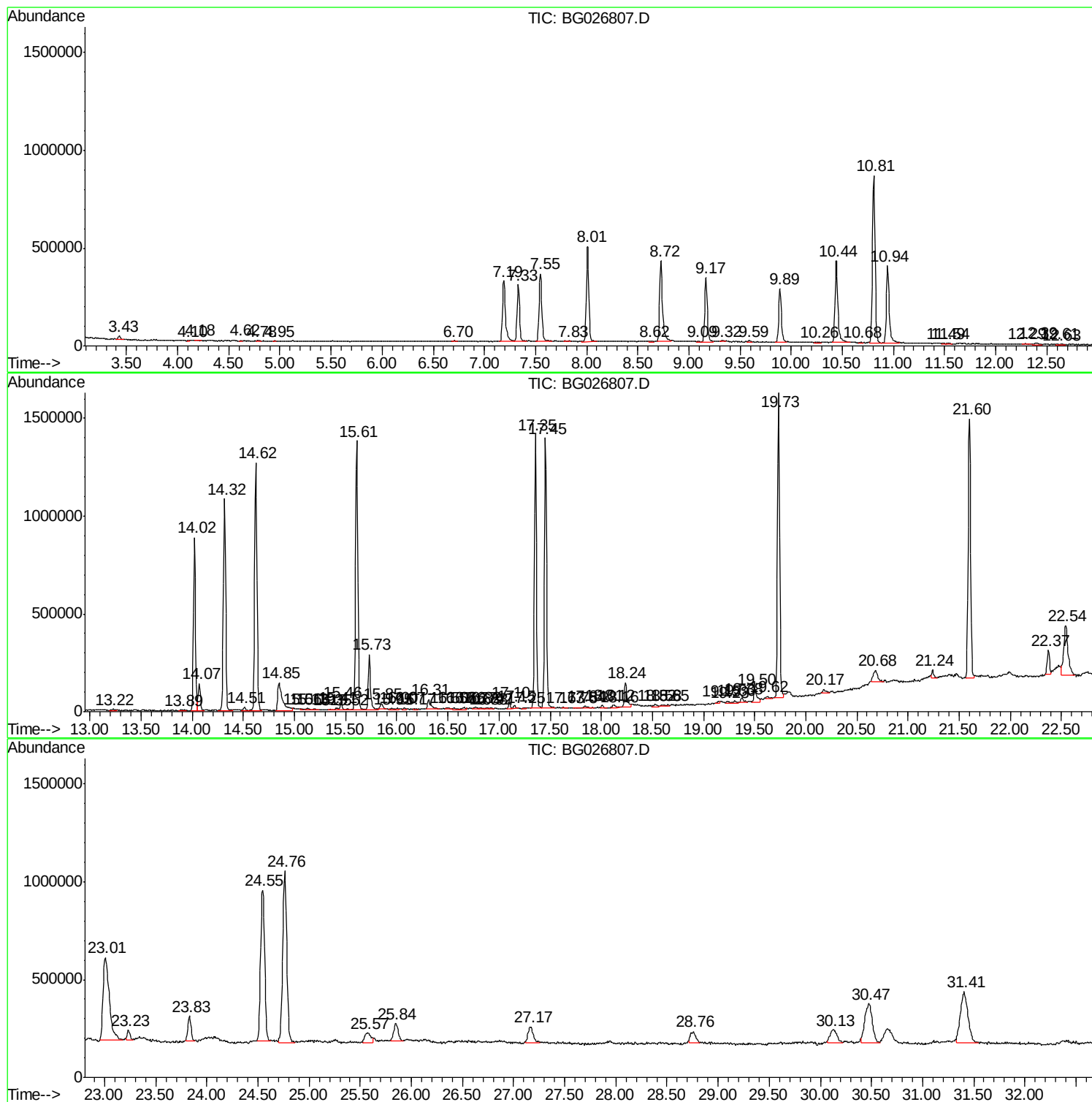
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Quant Title : SVOA CALIBRATION

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



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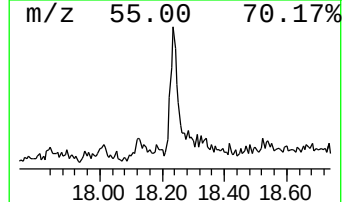
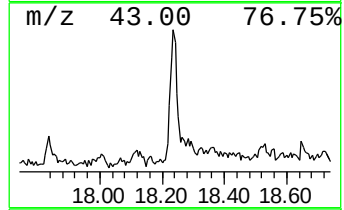
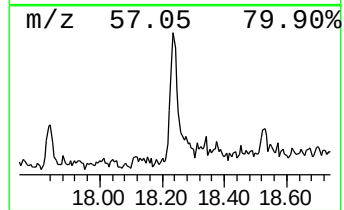
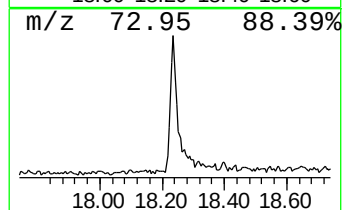
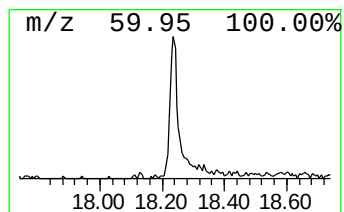
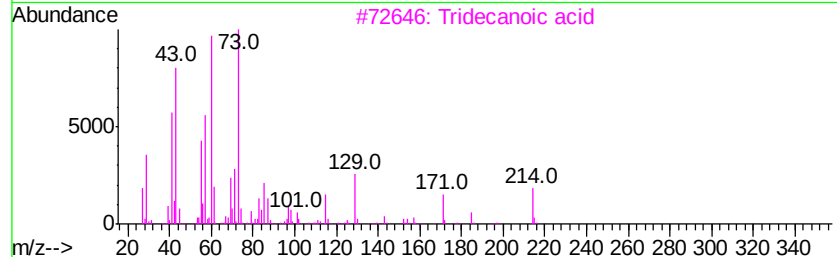
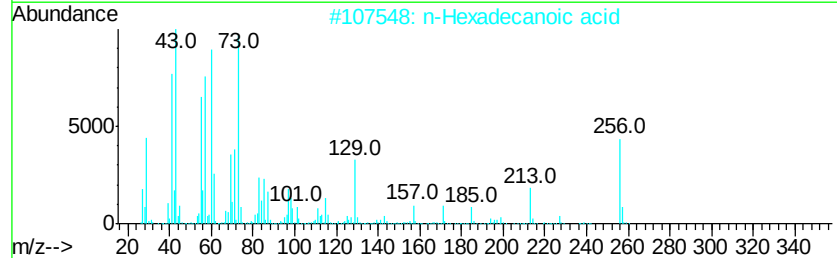
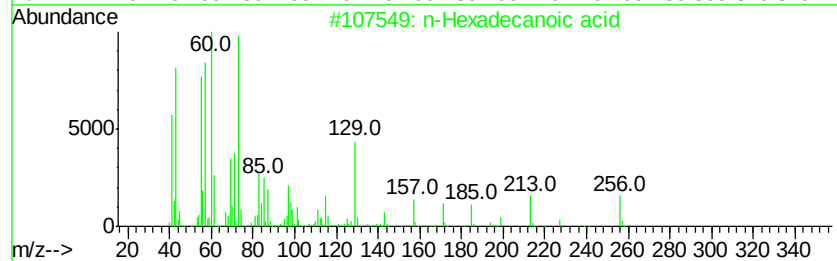
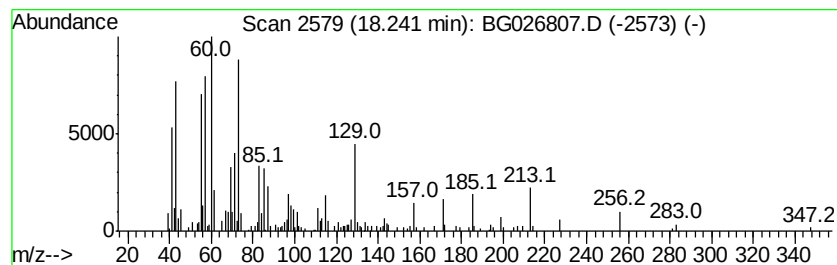
Instrument :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.24	2.19 ng/ul	225227	Phenanthrene-d10	17.35		
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	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Octadecanoic acid	284	C18H36O2	000057-11-4	81



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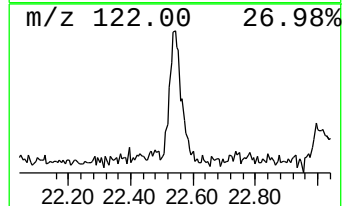
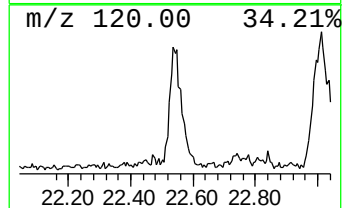
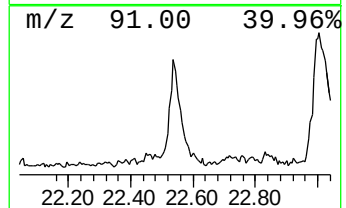
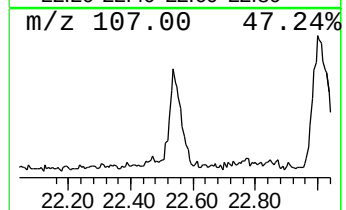
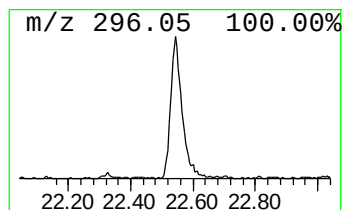
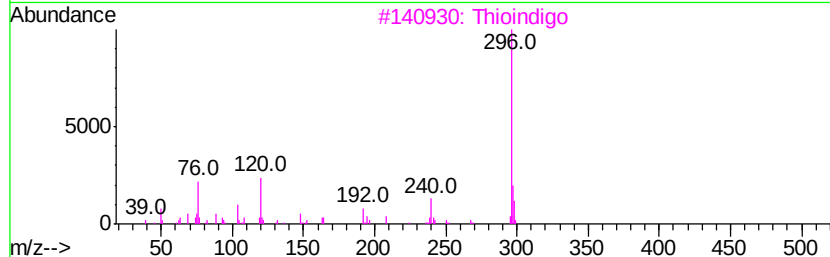
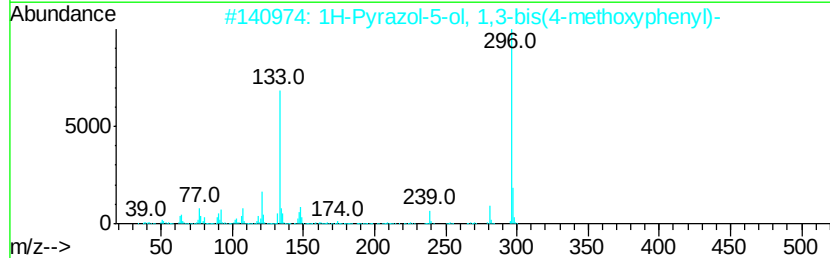
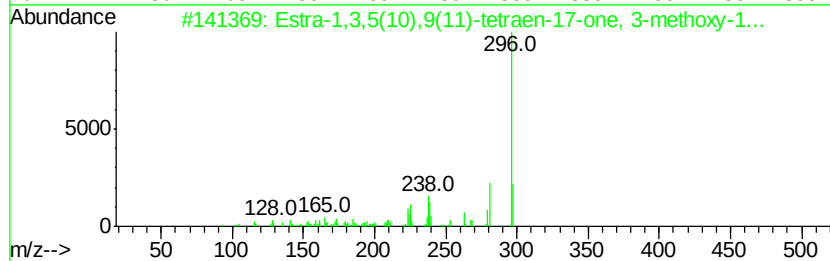
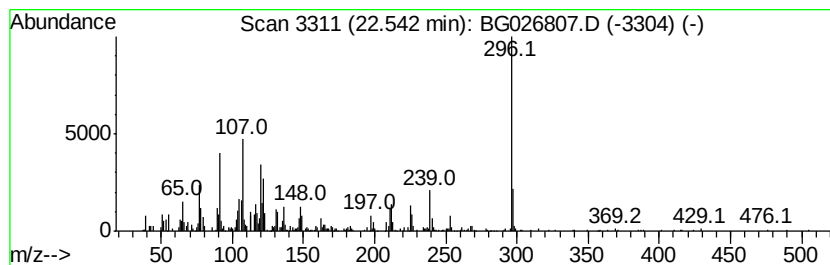
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Estra-1,3,5(10),9(11)-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	6.81 ng/ul	732762	Chrysene-d12	21.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estra-1,3,5(10),9(11)-tetraen-17...	296	C20H24O2	069796-63-0	50		
2	1H-Pyrazol-5-ol, 1,3-bis(4-metho...	296	C17H16N2O3	1000337-80-1	50		
3	Thioindigo	296	C16H8O2S2	000522-75-8	46		
4	3,5,7-Pregnatrien-20-one	296	C21H28O	1000227-49-1	38		
5	Pyrazol-5(4H)-one, 4-(2-fluoroph...	296	C16H13FN4O	125910-81-8	38		



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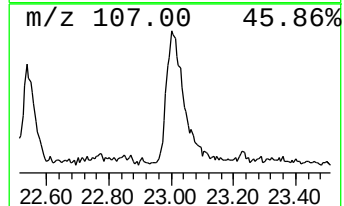
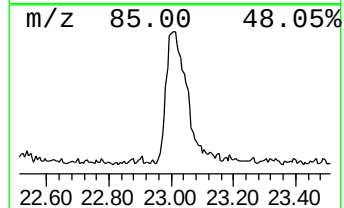
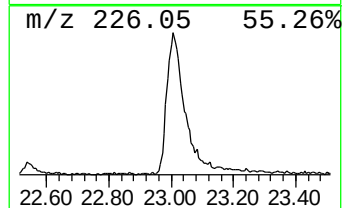
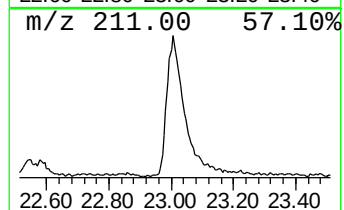
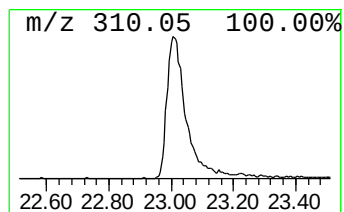
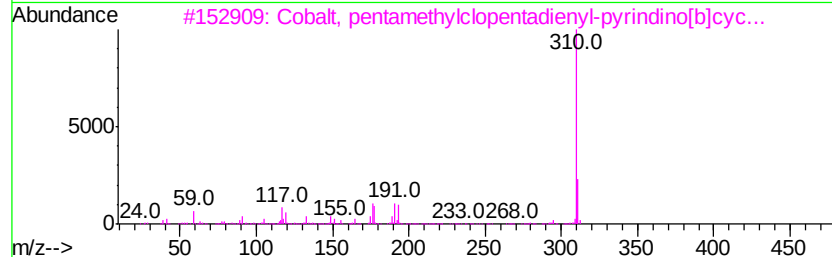
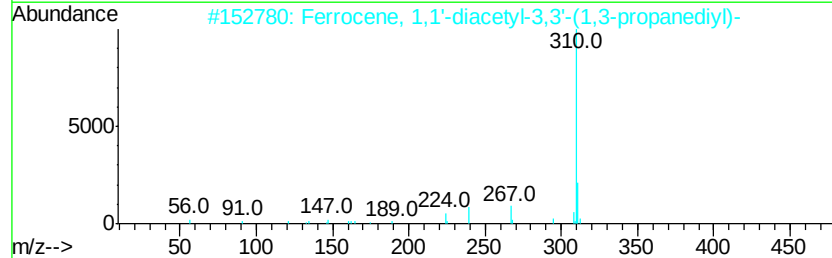
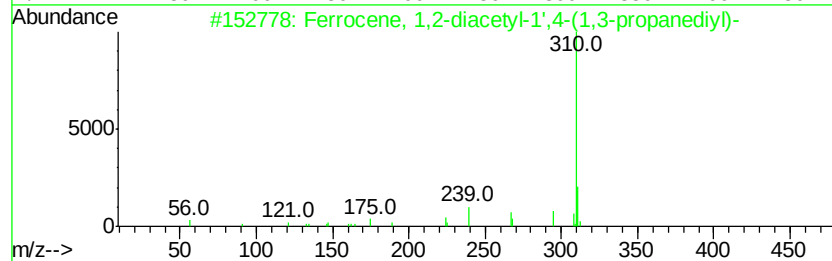
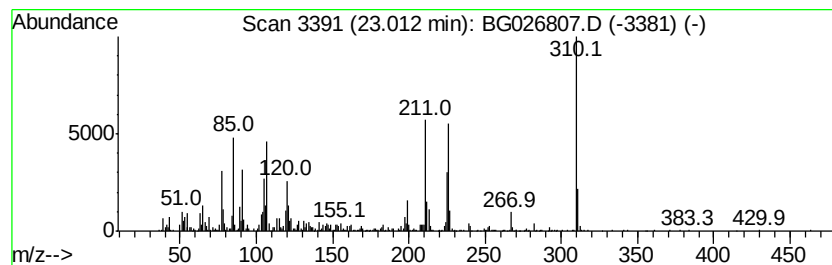
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	16.49 ng/ul	1773520	Chrysene-d12	21.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ferrocene, 1,2-diacetyl-1',4-(1,...	310	C17H18FeO2	041558-93-4	30
2		Ferrocene, 1,1'-diacetyl-3,3'-(1...	310	C17H18FeO2	041558-92-3	25
3		Cobalt, pentamethylclopentadienyl...	310	C18H21CoN	1000155-23-0	20
4		Beta-carboline, 6-methoxy-1,2-di...	226	C14H14N2O	154505-42-7	18
5		Xanthine, 2,4,7-trimethyl-8-[2-...	310	C17H18N4O2	1000129-52-8	18



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
Data File : BG026807.D
Acq On : 1 May 2017 15:18
Operator : SJ/MA
Sample : I2850-03
Misc :
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Instrument :
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ClientSampleId :
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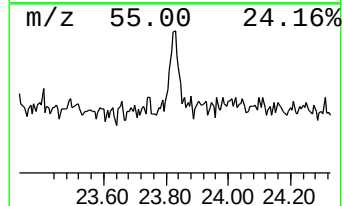
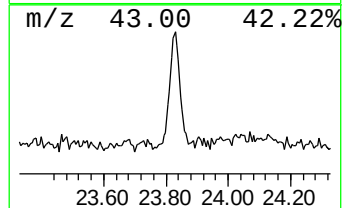
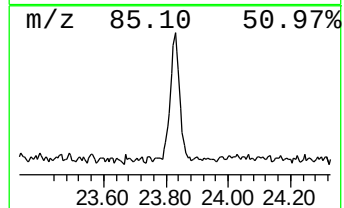
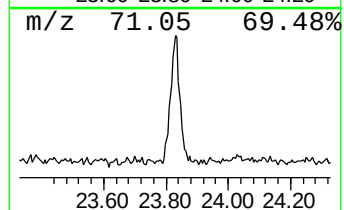
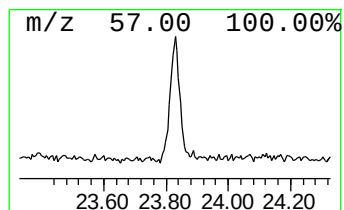
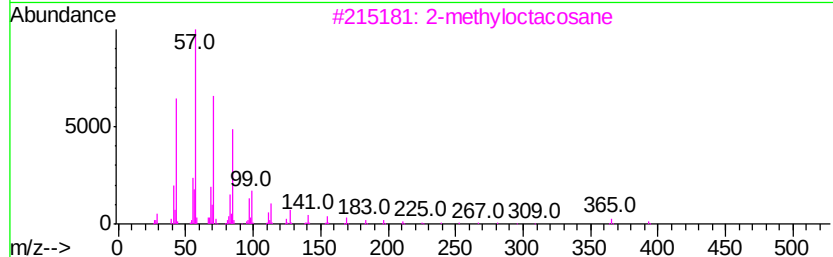
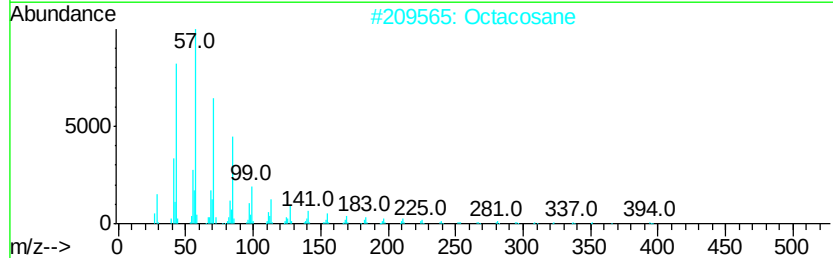
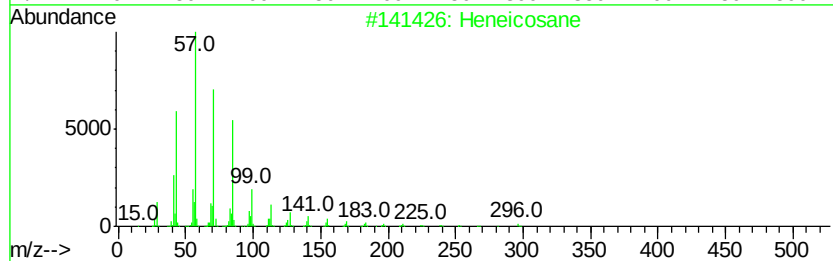
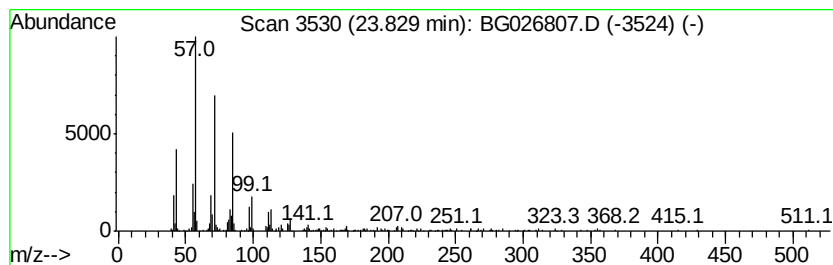
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.83	2.14 ng/ul	263792	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	93
2		Octacosane	394	C28H58	000630-02-4	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5		Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
Data File : BG026807.D
Acq On : 1 May 2017 15:18
Operator : SJ/MA
Sample : I2850-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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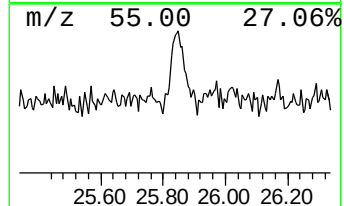
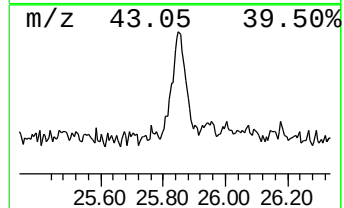
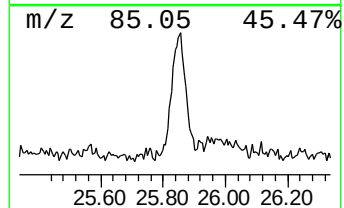
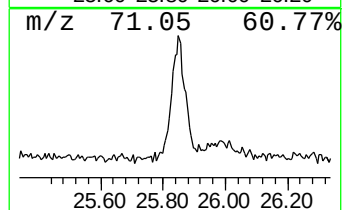
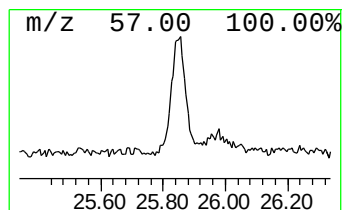
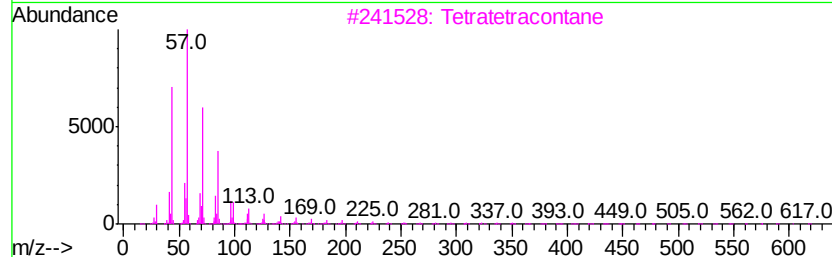
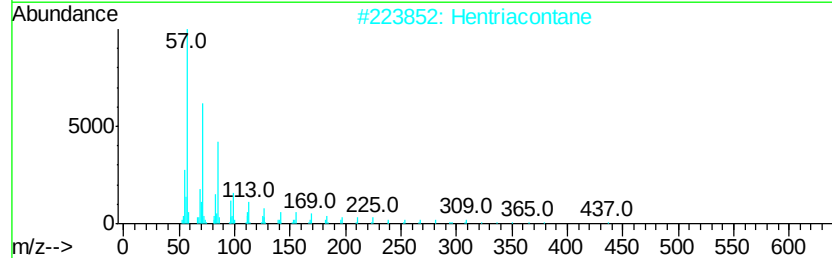
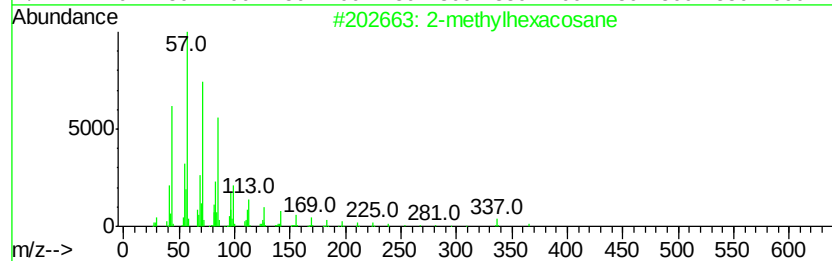
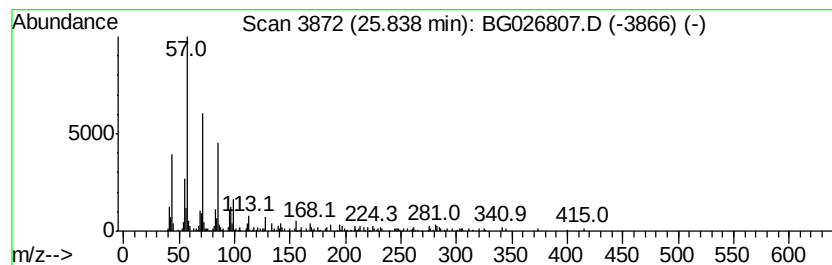
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.84	2.19 ng/ul	269524	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methylhexacosane	380	C27H56	1000376-72-7	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
Data File : BG026807.D
Acq On : 1 May 2017 15:18
Operator : SJ/MA
Sample : I2850-03
Misc :
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Instrument :
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ClientSampleId :
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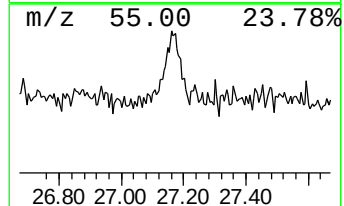
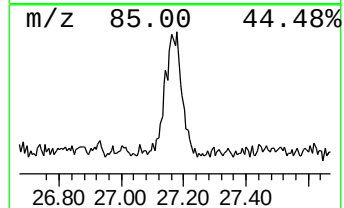
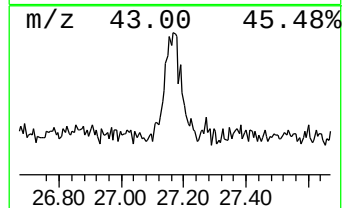
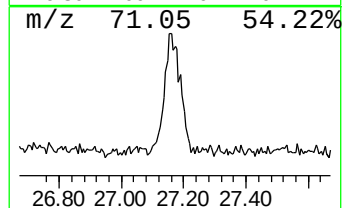
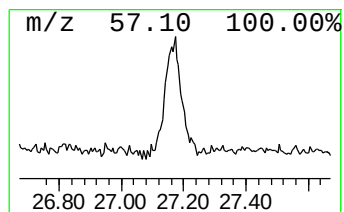
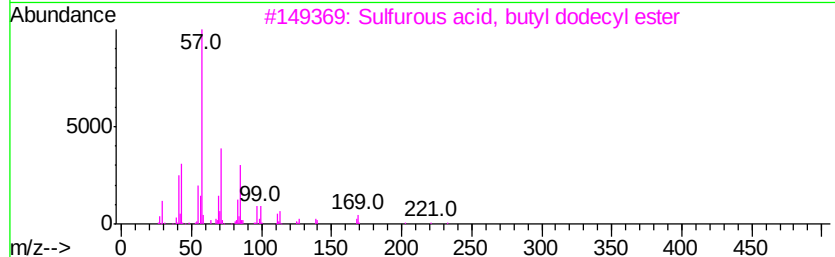
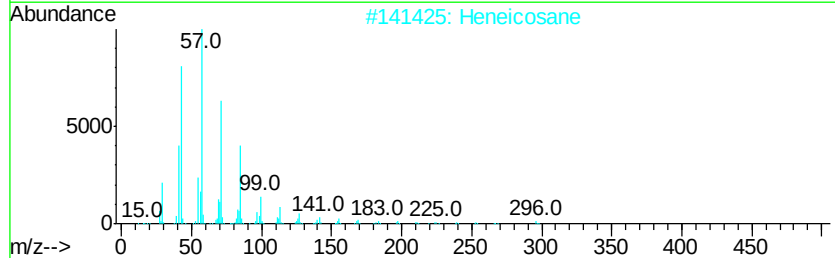
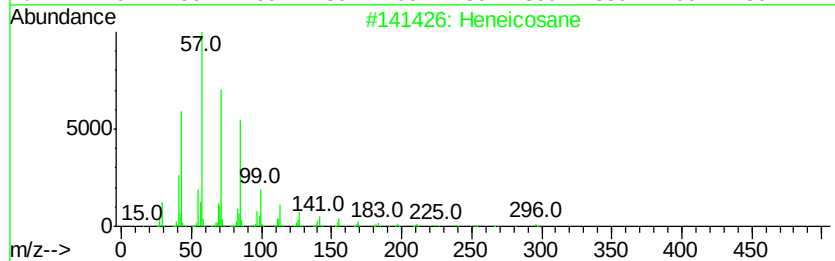
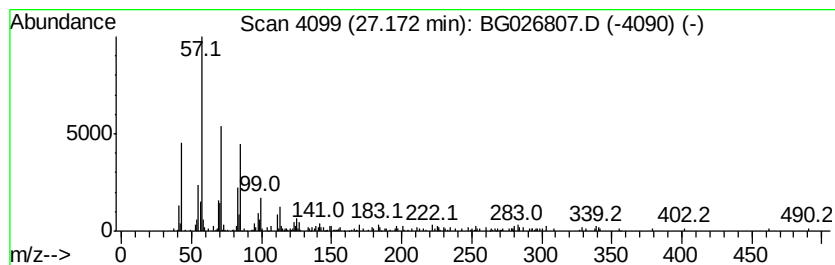
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.17	2.35 ng/ul	288724	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Heneicosane	296	C21H44	000629-94-7	89
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5		Tritetracontane	605	C43H88	007098-21-7	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
Data File : BG026807.D
Acq On : 1 May 2017 15:18
Operator : SJ/MA
Sample : I2850-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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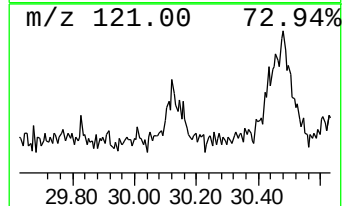
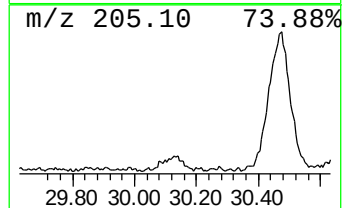
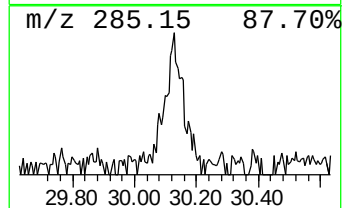
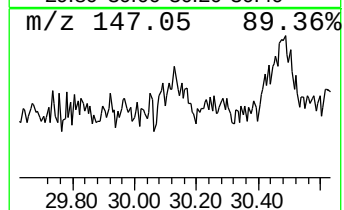
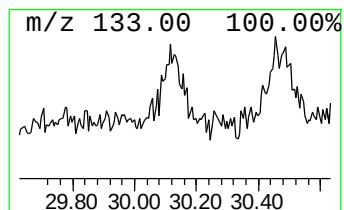
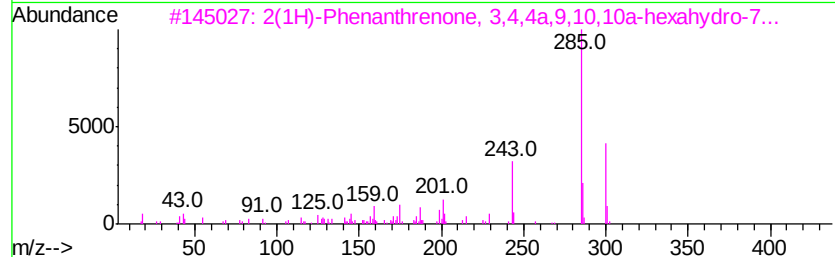
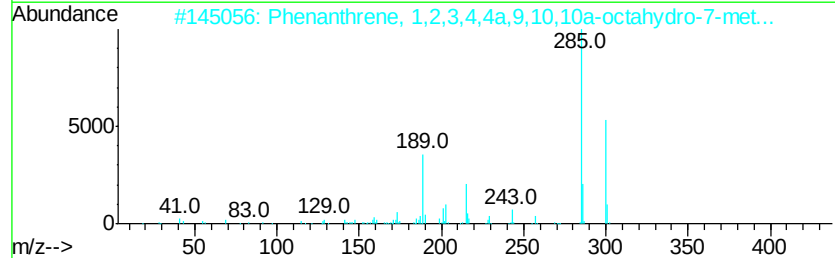
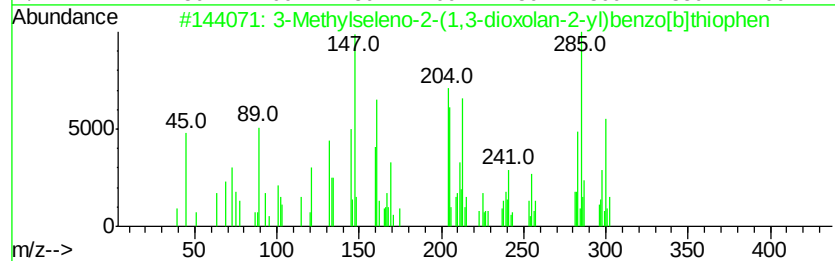
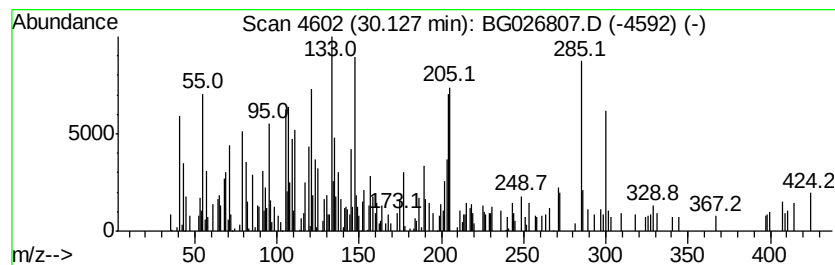
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 3-Methylseleno-2-(1,3-dioxo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.13	2.45 ng/ul	301531	Perylene-d12	24.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methylseleno-2-(1,3-dioxolan-2...	300	C12H12O2SSe	071740-02-8	52
2		Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	015340-83-7	25
3		2(1H)-Phenanthrenone, 3,4,4a,9,1...	300	C20H28O2	006755-93-7	25
4		Pyrido[3,4-d]pyridazin-1(2H)-one...	205	C9H11N5O	1000271-08-5	15
5		Acetamide, 2-[[[6,7-dihydro-2,1,...	300	C15H16N4O3	1000319-88-7	15



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
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Acq On : 1 May 2017 15:18
Operator : SJ/MA
Sample : I2850-03
Misc :
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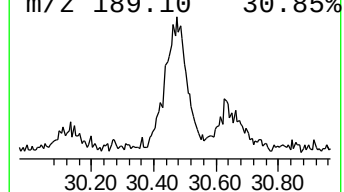
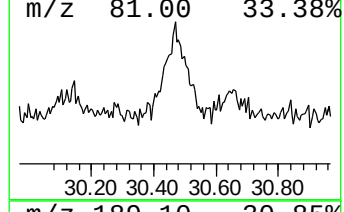
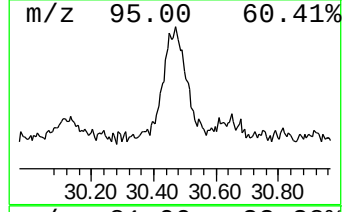
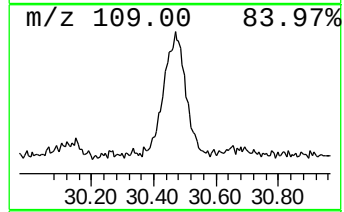
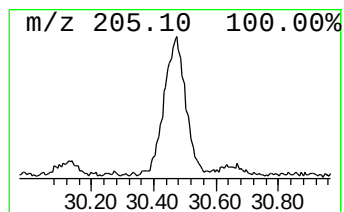
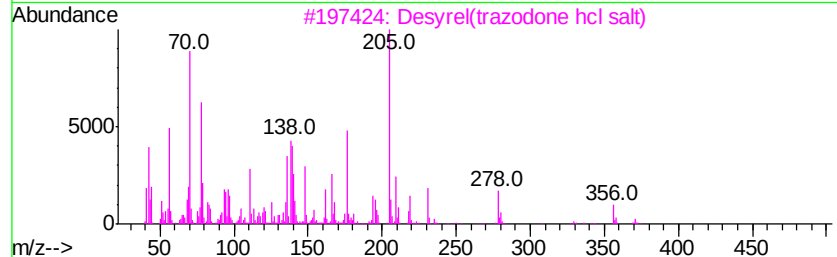
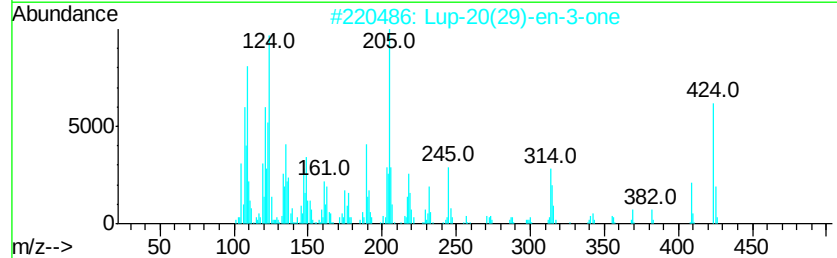
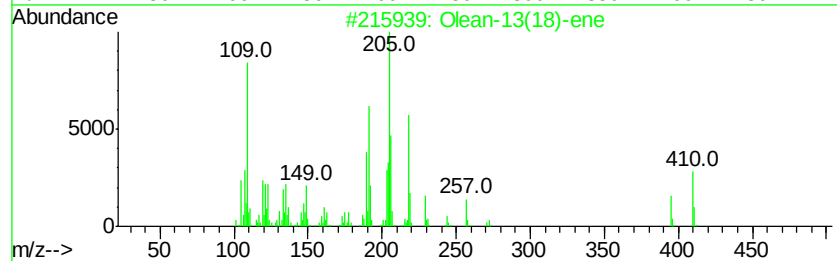
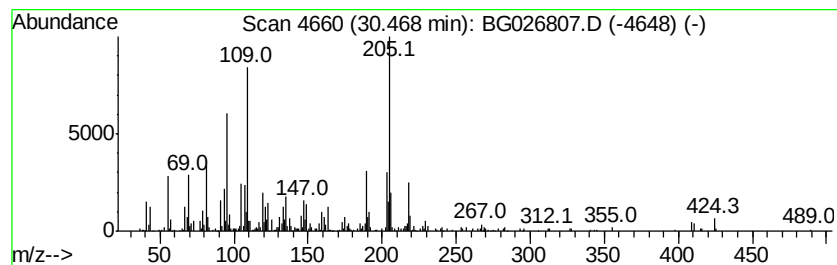
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG042717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 Olean-13(18)-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.47	8.05 ng/ul	991010	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Olean-13(18)-ene	410 C30H50	003399-27-7	70
2	Lup-20(29)-en-3-one	424 C30H48O	001617-70-5	38
3	Desvrel(trazodone hcl salt)	371 C19H22ClN5O	019794-93-5	35
4	1-Hydroxymethyl-5,8,9-endo-10-ex...	236 C16H28O	1000140-32-9	35
5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216 C6H5BrN2O2	300574-36-1	22



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050117\
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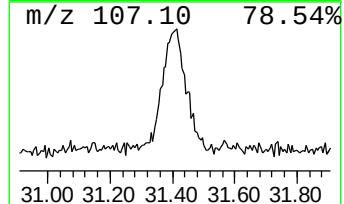
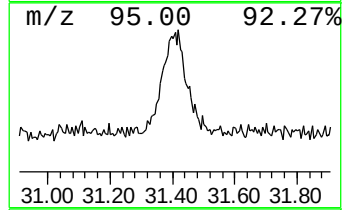
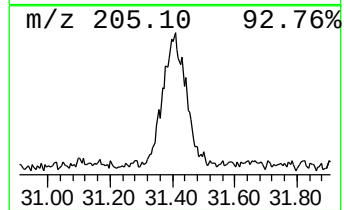
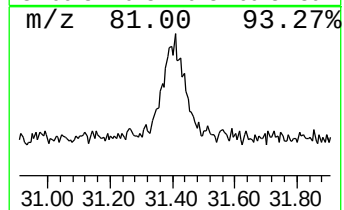
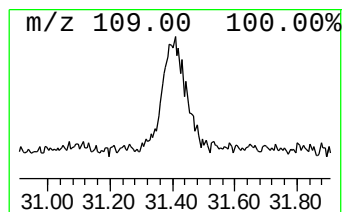
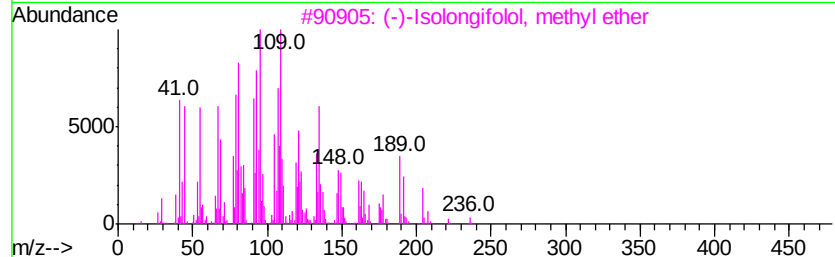
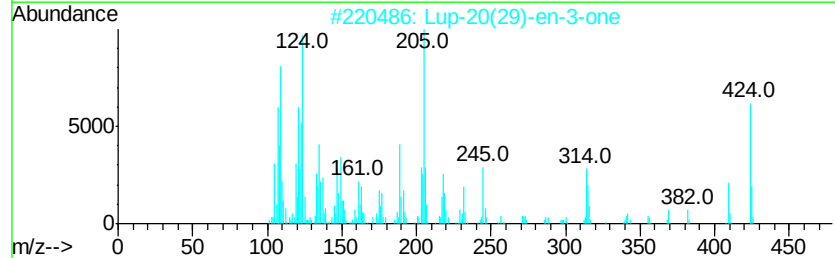
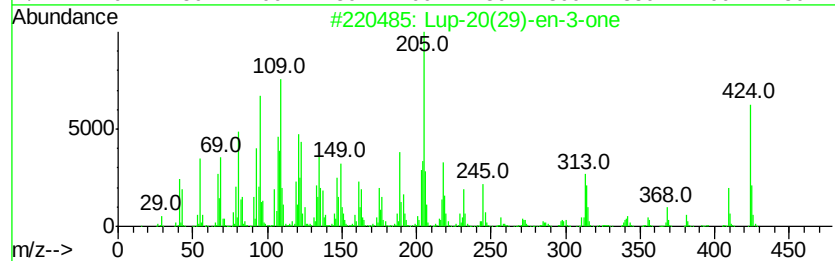
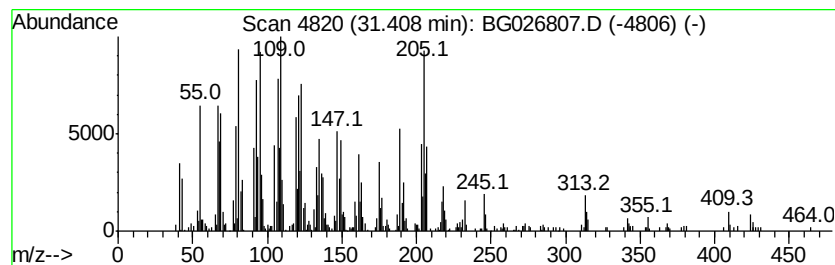
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.41	11.19 ng/ul	1376920	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Lup-20(29)-en-3-one	424 C30H48O	001617-70-5 86
2		Lup-20(29)-en-3-one	424 C30H48O	001617-70-5 86
3		(-)-Isolongifolol, methyl ether	236 C16H28O	1000333-80-8 50
4		But-3-enal, 2-methyl-4-(2,6,6-tr...	206 C14H22O	104900-59-6 49
5		D:C-Friedoolean-8-en-3-one	424 C30H48O	022611-26-3 46



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050117\
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Instrument :
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 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
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Estra-1,3,5(10),9...	22.54	6.8	ng/ul	732762	5	21.60	2150920	20.0
unknown-01	23.01	16.5	ng/ul	1773520	5	21.60	2150920	20.0
(DEL) Alkane: Str...	23.83	2.1	ng/ul	263792	6	24.76	2460950	20.0
(DEL) Alkane: Str...	25.84	2.2	ng/ul	269524	6	24.76	2460950	20.0
(DEL) Alkane: Str...	27.17	2.4	ng/ul	288724	6	24.76	2460950	20.0
3-Methylseleno-2-...	30.13	2.5	ng/ul	301531	6	24.76	2460950	20.0
Olean-13(18)-ene	30.47	8.1	ng/ul	991010	6	24.76	2460950	20.0
Lup-20(29)-en-3-one	31.41	11.2	ng/ul	1376920	6	24.76	2460950	20.0