LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.022	332	346	348	rBV2	14812	51103	2.41%	0.171%
2	4.745	466	469	472	rBV	82276	94826	4.48%	0.318%
3	4.934	490	501	504	rVV3	41302	139082	6.57%	0.466%
4	5.057	508	522	527	rVB3	31994	110844	5.24%	0.371%
5	5.198	543	546	557	rVB	192879	180077	8.51%	0.603%
6	5.392	566	579	585	rBV2	41651	110291	5.21%	0.369%
7	5.534	600	603	614	rVB	467179	486451	22.98%	1.630%
8	6.016	675	685	689	rBV	41152	83807	3.96%	0.281%
9	6.245	720	724	725	rBV	181577	205897	9.73%	0.690%
10	6.369	741	745	750	rBV	303533	270475	12.78%	0.906%
11	6.598	780	784	788	rBV	571021	452608	21.38%	1.516%
12	6.675	794	797	803	rBV	90638	78251	3.70%	0.262%
13	6.751	807	810	814	rVV	707706	637180	30.10%	2.135%
14	7.016	853	855	867	rVB	248289	248859	11.76%	0.834%
15	7.157	873	879	883	rBV	668793	542953	25.65%	1.819%
16	7.222	887	890	893	rVB	64406	53473	2.53%	0.179%
17	7.257	893	896	900	rBV	68287	59230	2.80%	0.198%
18	7.345	907	911	916	rBV	59068	59169	2.80%	0.198%
19	7.663	957	965	969	rBV	158568	215100	10.16%	0.721%
20	7.798	984	988	992	rBV	346512	275716	13.03%	0.924%
21	7.881	999	1002	1005	rVV	776674	605213	28.59%	2.027%
22	7.910	1005	1007	1010	rVV	81781	77499	3.66%	0.260%
23	8.039	1026	1029	1035	rBV	194759	195999	9.26%	0.657%
24	8.163	1044	1050	1054	rBV2	61524	90223	4.26%	0.302%
25	8.322	1075	1077	1081	rVB	58397	50837	2.40%	0.170%
26	8.522	1108	1111	1115	rVB	470587	343756	16.24%	1.152%
27	8.686	1136	1139	1149	rVB	74189	80354	3.80%	0.269%
28	8.828	1157	1163	1167	rVV2	226507	288621	13.64%	0.967%
29	8.957	1181	1185	1188	rBV	1368453	1040332	49.15%	3.485%
30	9.351	1249	1252	1256	rBV	196814	150544	7.11%	0.504%
31	9.451	1265	1269	1277	rVB	882885	721819	34.10%	2.418%
32	9.627	1293	1299	1302	rBV2	737052	871884	41.19%	2.921%
33	9.875	1333	1341	1344	rBV	500511	597492	28.23%	2.002%
34	9.963	1353	1356	1359	rBV	189411	157551	7.44%	0.528%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.163	1386	1390	1392	rVB	60062	56138	2.65%	0.188%
36	10.280	1408	1410	1414	rBV2	88529	83666	3.95%	0.280%
37	10.345	1418	1421	1425	rVV	74024	76446	3.61%	0.256%
38	10.410	1429	1432	1435	rBV	159695	157511	7.44%	0.528%
39	10.451	1435	1439	1443	rVV	640292	599303	28.31%	2.008%
40	10.504	1443	1448	1449	rVV5	56349	83089	3.93%	0.278%
41	10.551	1453	1456	1458	rVV	83141	89956	4.25%	0.301%
42	10.580	1458	1461	1464	rVV	353942	352442	16.65%	1.181%
43	10.639	1467	1471	1479	rVB	308582	301363	14.24%	1.010%
44	10.804	1496	1499	1503	rVV	251175	230778	10.90%	0.773%
45	10.910	1514	1517	1522	rVB	275811	245820	11.61%	0.823%
46	10.957	1522	1525	1528	rVV	56211	52856	2.50%	0.177%
47	10.992	1528	1531	1534	rVB2	49659	51689	2.44%	0.173%
48	11.104	1541	1550	1556	rBV	508154	538403	25.44%	1.804%
49	11.239	1569	1573	1577	rBV4	44875	63723	3.01%	0.213%
50	11.286	1577	1581	1586	rVB	363908	291291	13.76%	0.976%
51	11.345	1588	1591	1598	rBV	641806	621646	29.37%	2.082%
52	11.457	1607	1610	1614	rBV	151749	154714	7.31%	0.518%
53	11.521	1618	1621	1625	rVB	160460	133089	6.29%	0.446%
54	11.680	1640	1648	1661	rBV	1464917	2046641	96.69%	6.856%
55	11.810	1667	1670	1678	rVB2	67391	77629	3.67%	0.260%
56	11.904	1683	1686	1689	rVV	85776	75537	3.57%	0.253%
57	11.933	1689	1691	1697	rVB3	65766	73548	3.47%	0.246%
58	12.080	1713	1716	1723	rVV5	64860	126444	5.97%	0.424%
59	12.163	1727	1730	1736	rBV	478810	445549	21.05%	1.493%
60	12.245	1741	1744	1748	rVB2	67645	79321	3.75%	0.266%
61	12.310	1752	1755	1759	rBV3	67222	99608	4.71%	0.334%
62	12.380	1759	1767	1769	rVV	751145	1114925	52.67%	3.735%
63	12.404	1769	1771	1775	rVV	423223	483803	22.86%	1.621%
64	12.457	1775	1780	1789	rVV	922990	1281647	60.55%	4.293%
65	12.539	1790	1794	1799	rVV4	124329	218209	10.31%	0.731%
66	12.586	1799	1802	1809	rVB3	95622	138478	6.54%	0.464%
67	12.686	1815	1819	1822	rBV	746333	645157	30.48%	2.161%
68	12.839	1841	1845	1850	rVB3	77045	99090	4.68%	0.332%
69	12.910	1854	1857	1860	rBV2	53268	63537	3.00%	0.213%
70	13.180	1900	1903	1907	rVB3	63296	71862	3.40%	0.241%
71	13.527	1957	1962	1966	rBV4	81059	110149	5.20%	0.369%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.604	1970	1975	1978	rBV3	130956	168874	7.98%	0.566%
73	13.639	1978	1981	1989	rVB	128167	146034	6.90%	0.489%
74	13.727	1993	1996	1999	rBV	469604	396301	18.72%	1.328%
75	14.074	2051	2055	2059	rVB3	54226	61927	2.93%	0.207%
76	14.133	2062	2065	2069	rBV2	73043	74988	3.54%	0.251%
77	14.221	2077	2080	2086	rVB	72355	76702	3.62%	0.257%
78	14.374	2103	2106	2110	rVB	240674	212313	10.03%	0.711%
79	14.421	2111	2114	2120	rBV4	71309	90365	4.27%	0.303%
80	14.486	2122	2125	2128	rVV	130615	121862	5.76%	0.408%
81	14.515	2128	2130	2133	rVB	65987	57622	2.72%	0.193%
82	14.580	2137	2141	2145	rBV	934654	861923	40.72%	2.887%
83	14.674	2154	2157	2158	rBV2	54493	62212	2.94%	0.208%
84	14.733	2162	2167	2174	rVB2	159731	215548	10.18%	0.722%
85	14.815	2178	2181	2184	rBV2	66261	65373	3.09%	0.219%
86	14.845	2184	2186	2190	rVB4	92176	95350	4.50%	0.319%
87	15.004	2210	2213	2216	rVB3	86112	98274	4.64%	0.329%
88	15.039	2216	2219	2225	rVB2	99202	121116	5.72%	0.406%
89	15.098	2225	2229	2235	rBV	237897	269668	12.74%	0.903%
90	15.404	2278	2281	2284	rBV4	45018	54807	2.59%	0.184%
91	15.727	2330	2336	2349	rBV5	805805	1809948	85.51%	6.063%
92	15.821	2349	2352	2356	rVB2	62105	85882	4.06%	0.288%
93	15.886	2357	2363	2371	rBV3	1032635	2116669	100.00%	7.091%
94	16.409	2449	2452	2461	rVB9	52940	107292	5.07%	0.359%
95	16.533	2469	2473	2486	rVB3	93031	207821	9.82%	0.696%
96	16.698	2495	2501	2507	rBV4	94990	209244	9.89%	0.701%
97	16.768	2507	2513	2525	rVV3	121014	302940	14.31%	1.015%
98	16.898	2528	2535	2546	rVB10	174248	545767	25.78%	1.828%
99	18.180	2748	2753	2754	rBV4	68381	91870	4.34%	0.308%
100	18.339	2776	2780	2785	rVB7	34898	59797	2.83%	0.200%

Sum of corrected areas: 29851062

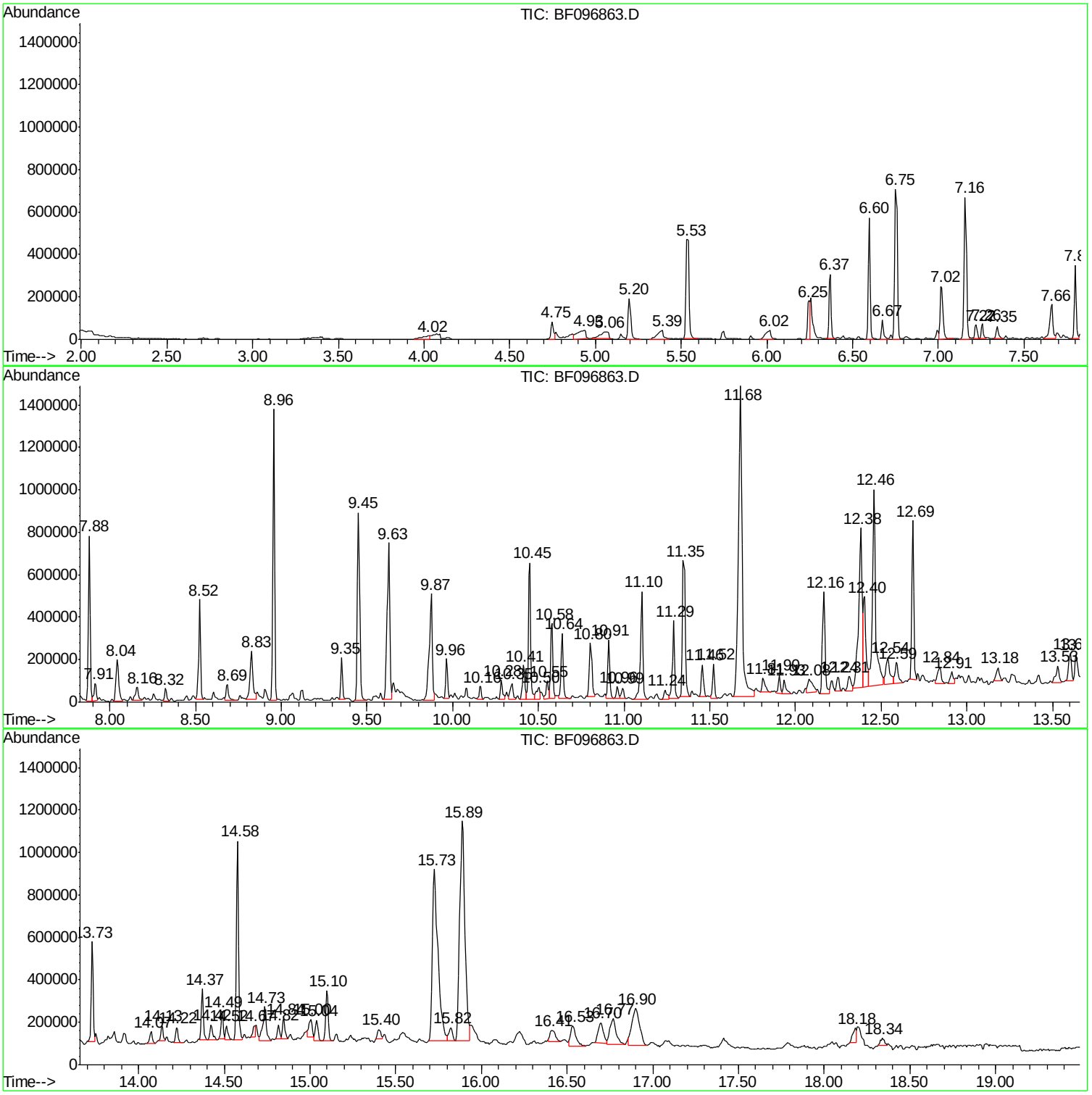
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

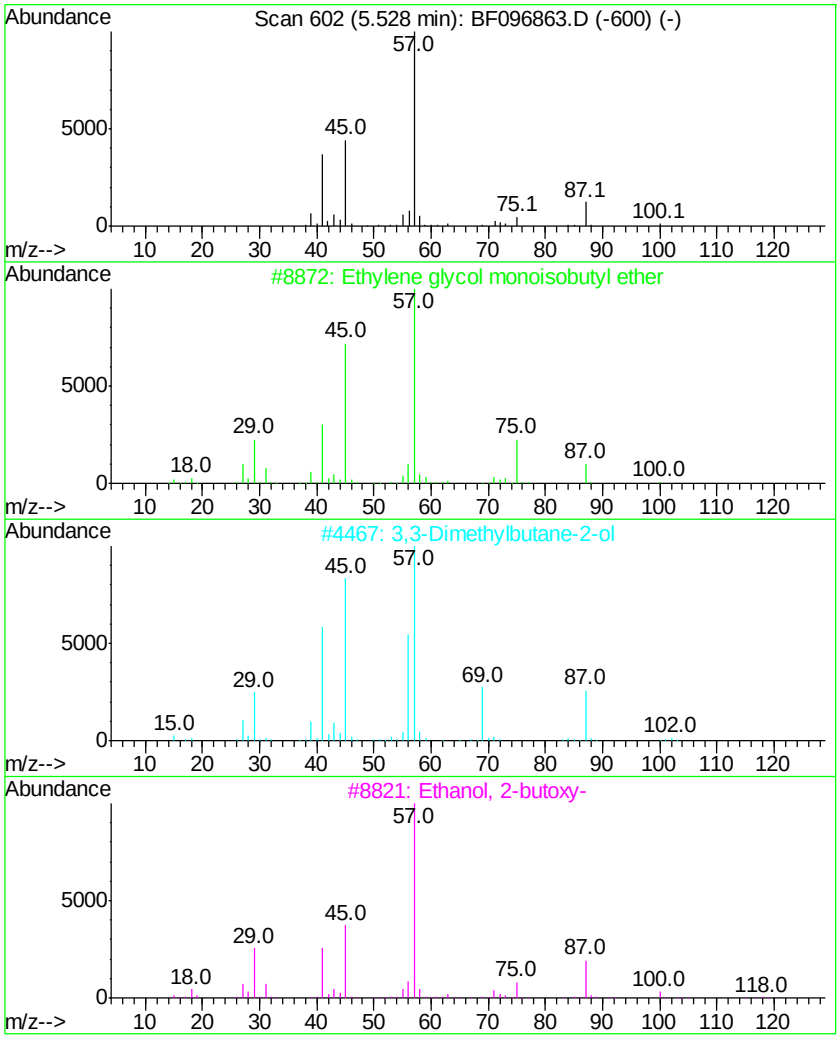
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

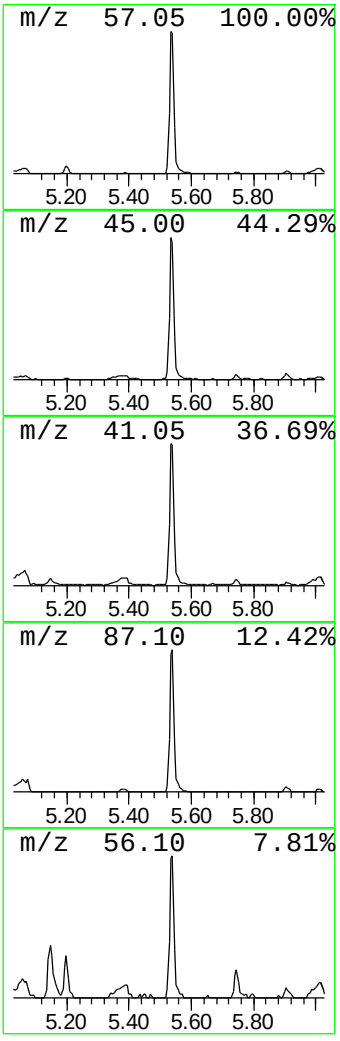
****

Peak Number 1 Ethylene glycol monoisobuty... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	21.50 ng	486451	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47
4	n-Butyl ether	130	C8H18O	000142-96-1	27
5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

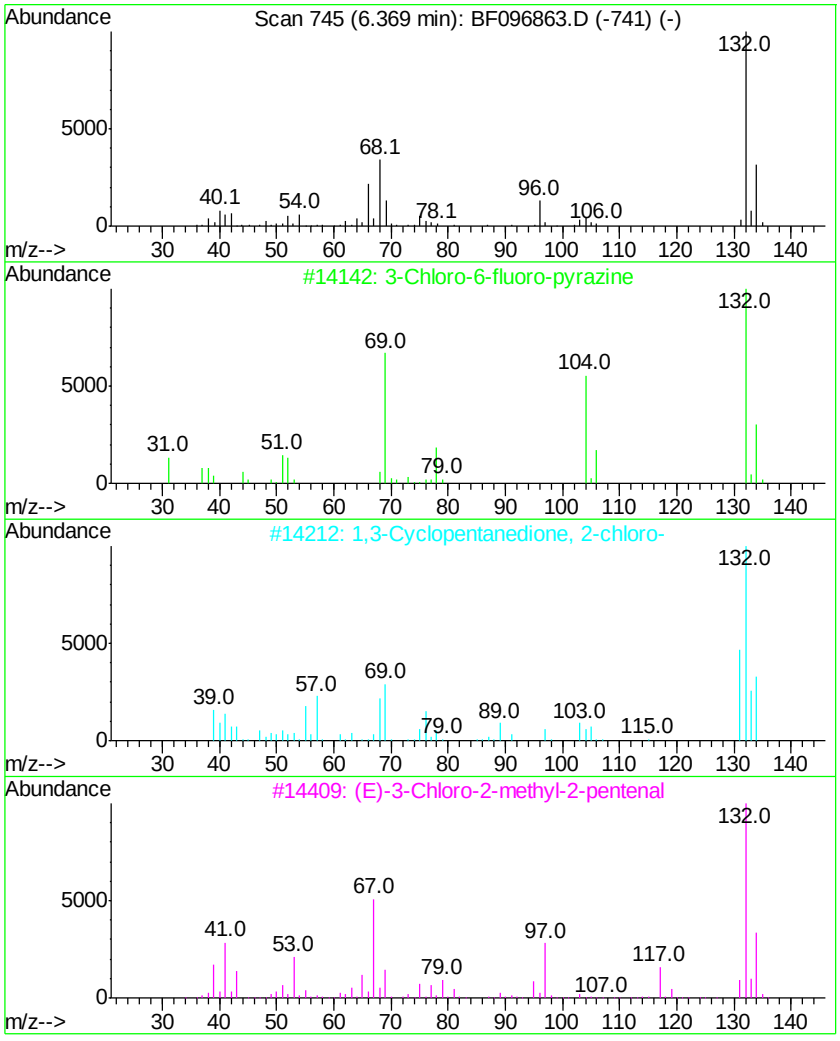
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

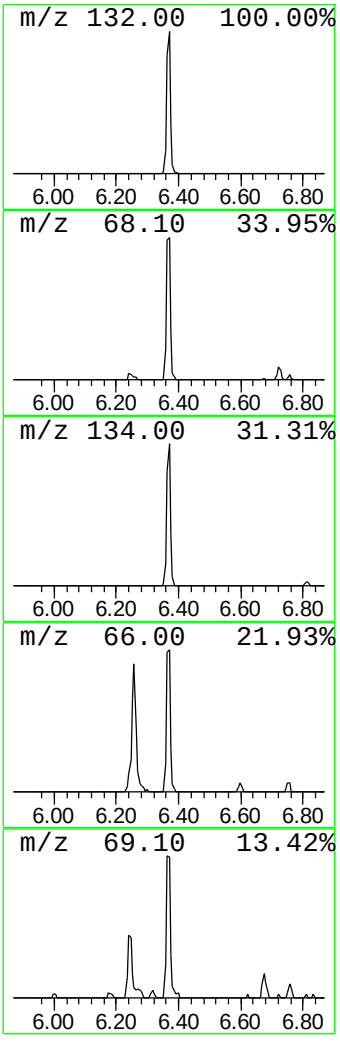
****

Peak Number 2 unknown6.37 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	11.95 ng	270475	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

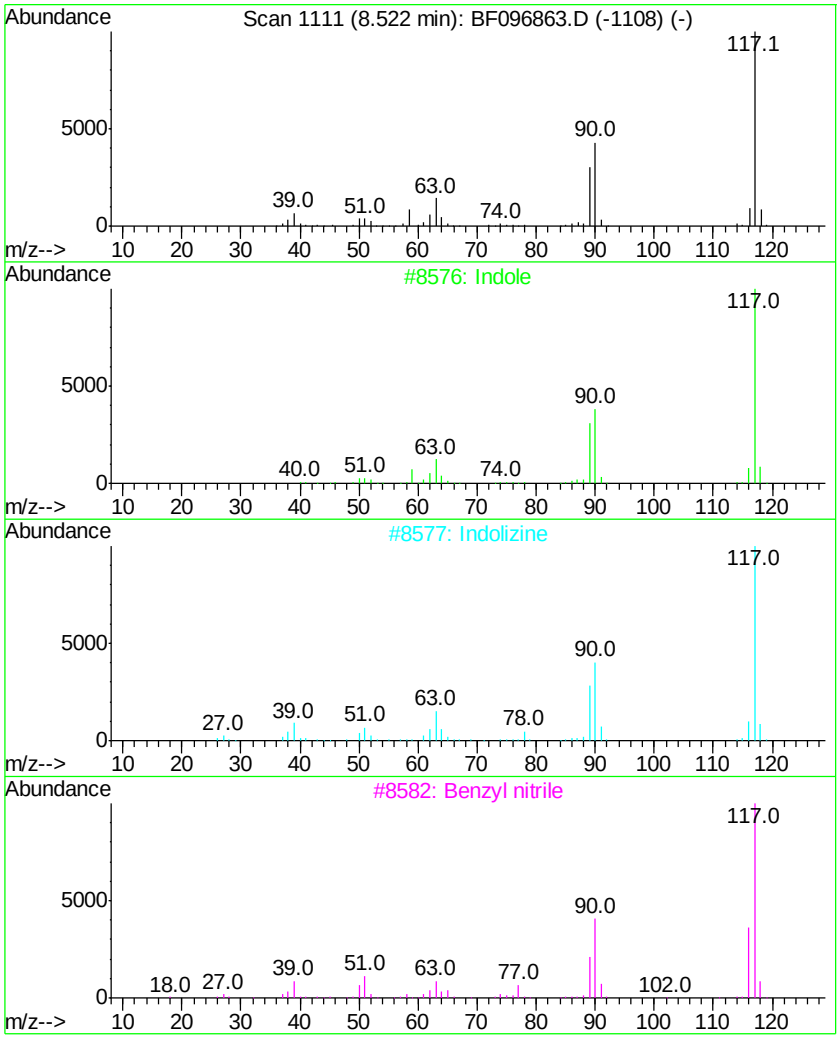
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

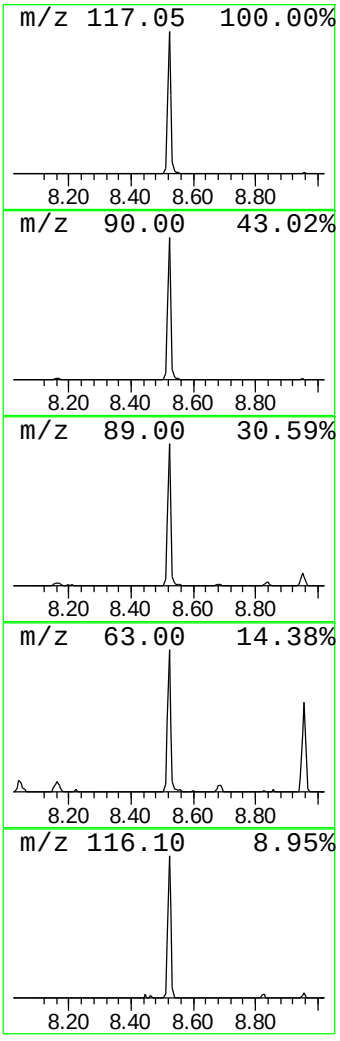
****

Peak Number 3 Indole Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	11.36 ng	343756	Naphthalene-d8	7.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	97
2	Indolizine	117	C8H7N	000274-40-8	94
3	Benzyl nitrile	117	C8H7N	000140-29-4	91
4	m-Aminophenylacetylene	117	C8H7N	054060-30-9	87
5	Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

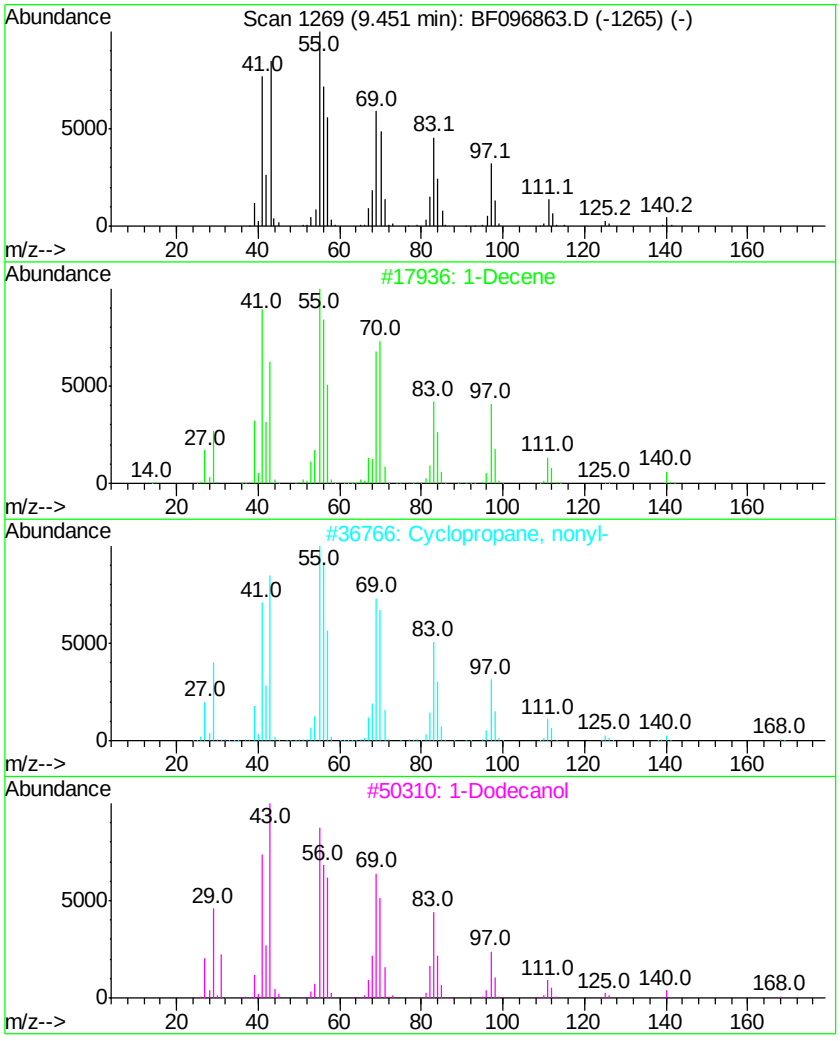
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

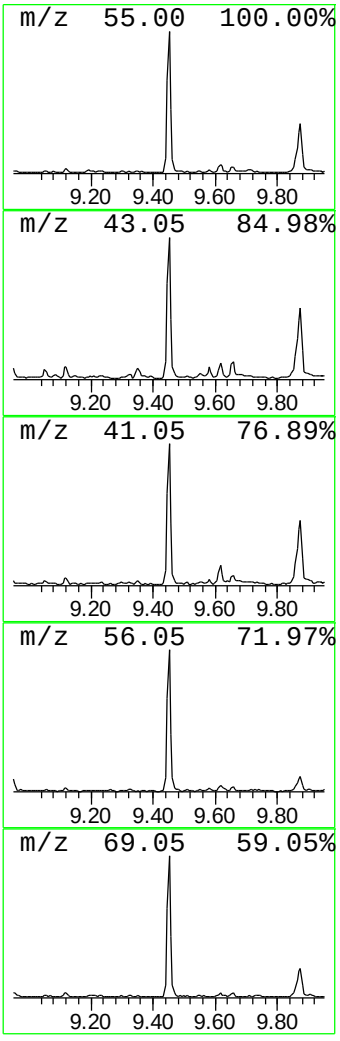
****

Peak Number 4 1-Decene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	16.56 ng	721819	Acenaphthene-d10	9.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene	140	C10H20	000872-05-9	94
2	Cyclopropane, nonyl-	168	C12H24	074663-85-7	91
3	1-Dodecanol	186	C12H26O	000112-53-8	91
4	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	90
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

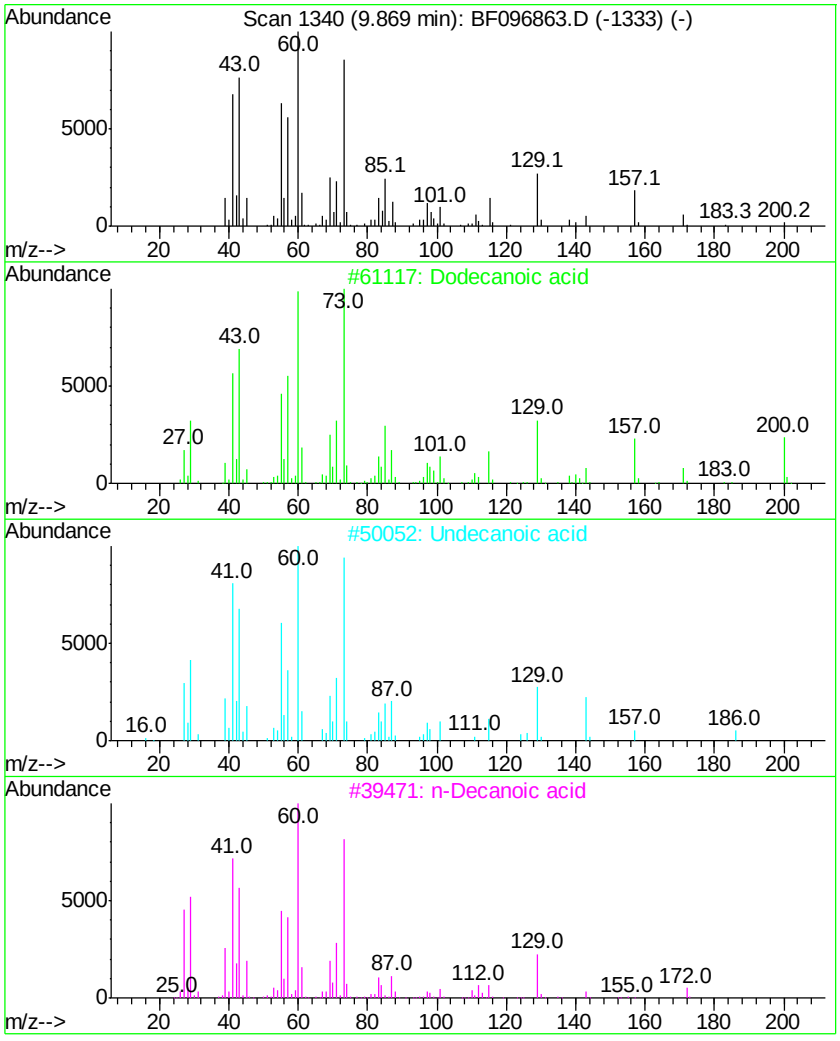
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

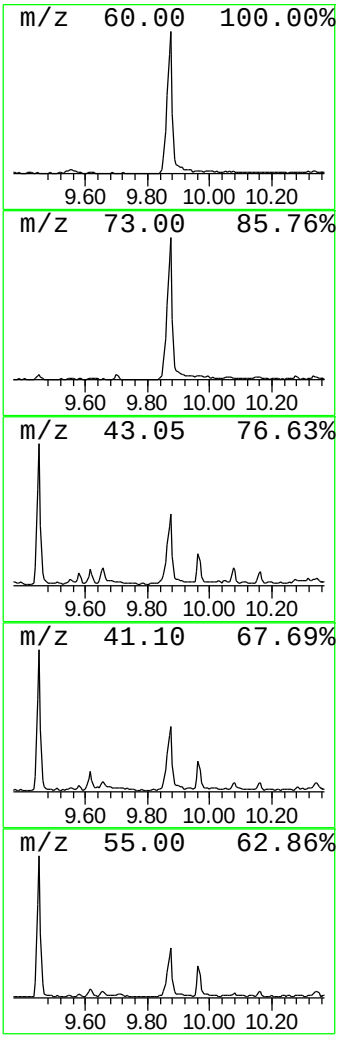
****

Peak Number 5 Dodecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	13.71 ng	597492	Acenaphthene-d10	9.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Nonanoic acid	158	C9H18O2	000112-05-0	58
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

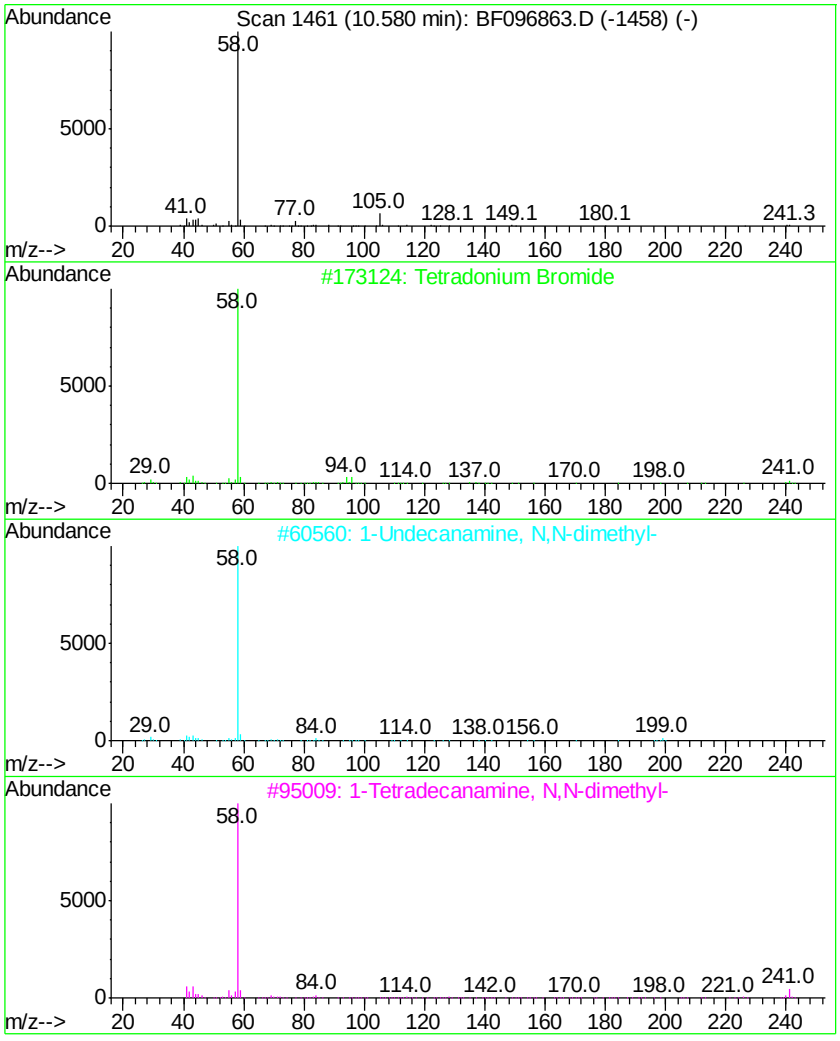
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

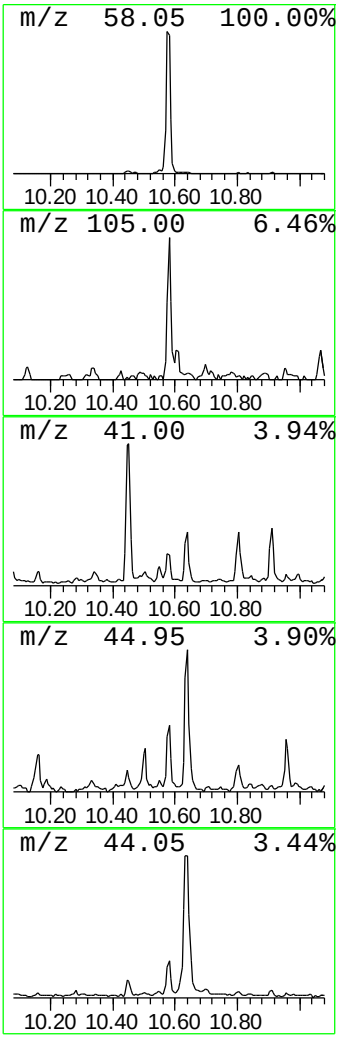
****

Peak Number 6 Tetradonium Bromide Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	13.09 ng	352442	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradonium Bromide	335	C17H38BrN	001119-97-7	56
2	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	50
3	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	50
4	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	50
5	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

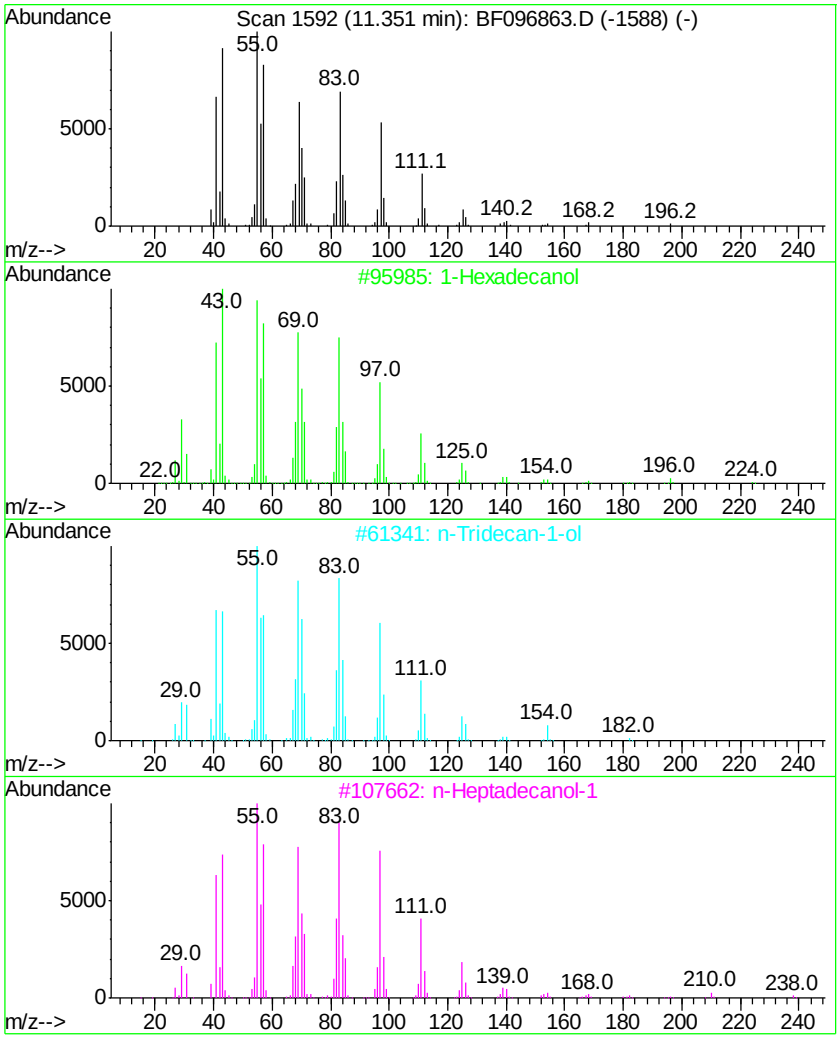
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

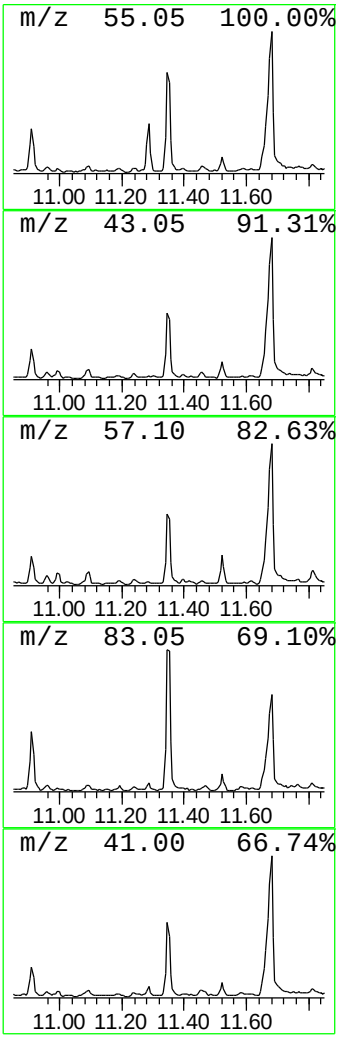
****

Peak Number 7 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	23.09 ng	621646	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	Cetene	224	C16H32	000629-73-2	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

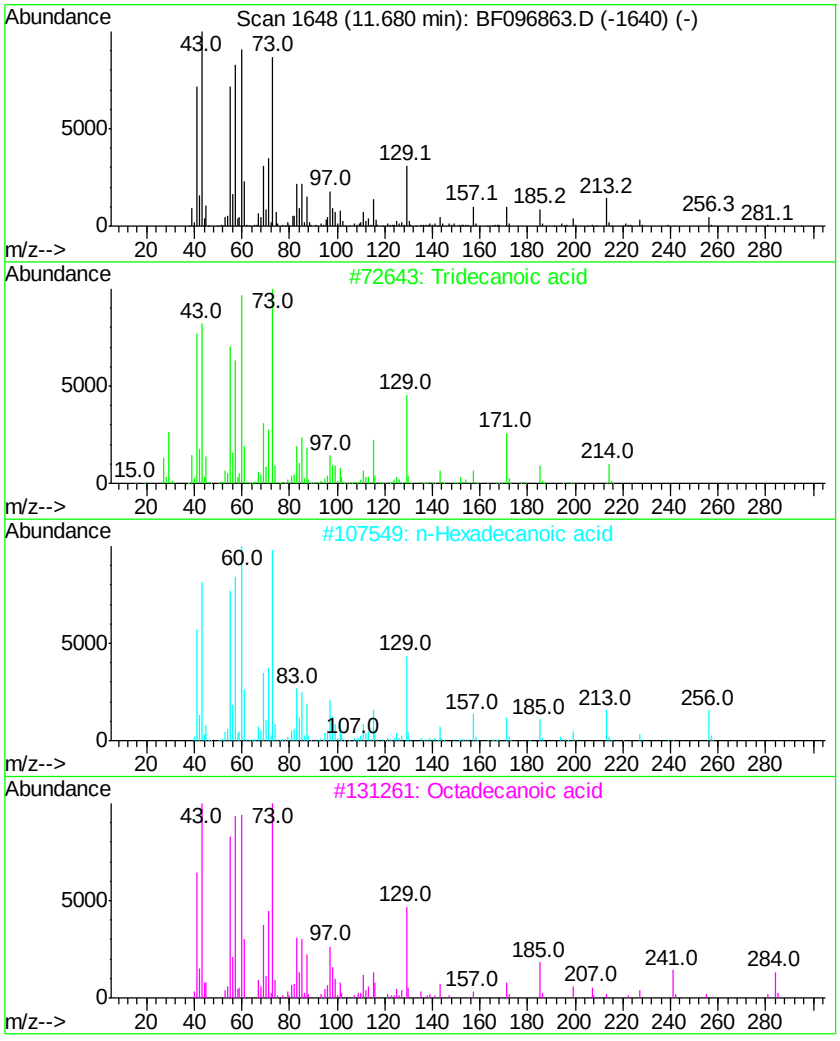
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

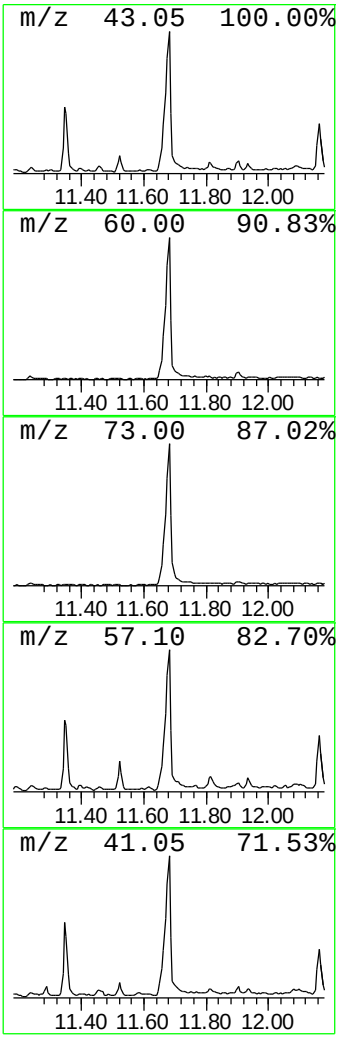
****

Peak Number 8 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	76.03 ng	2046640	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

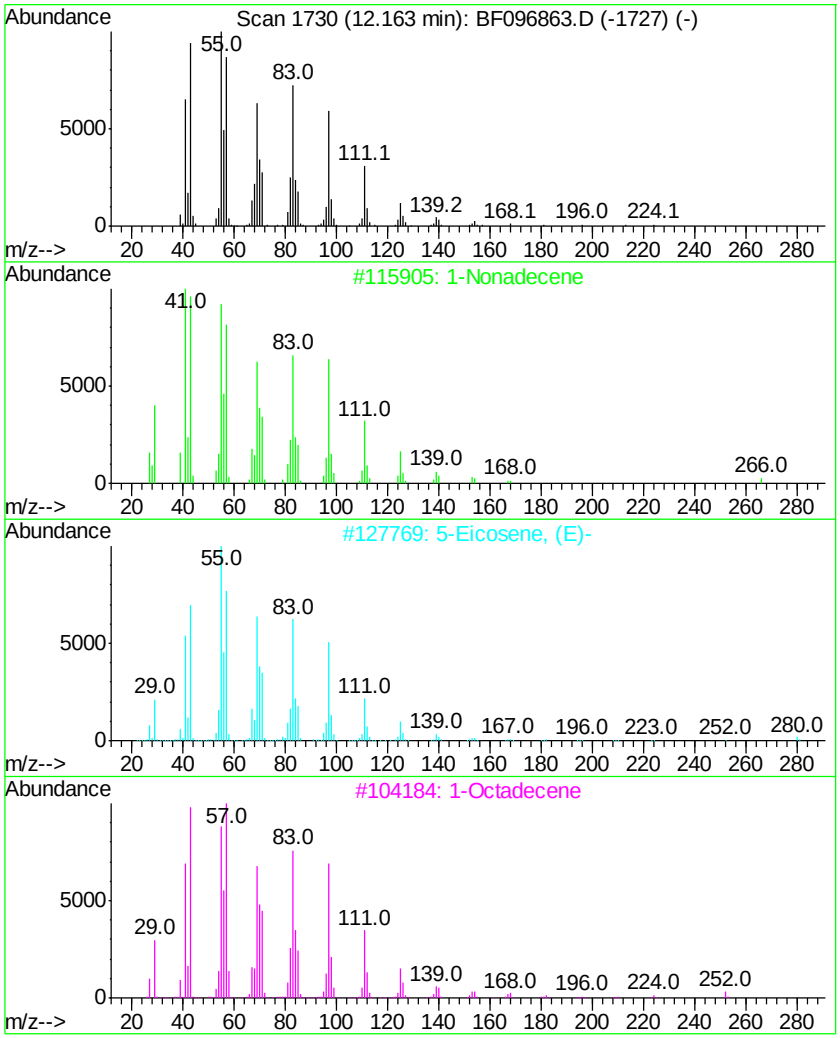
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

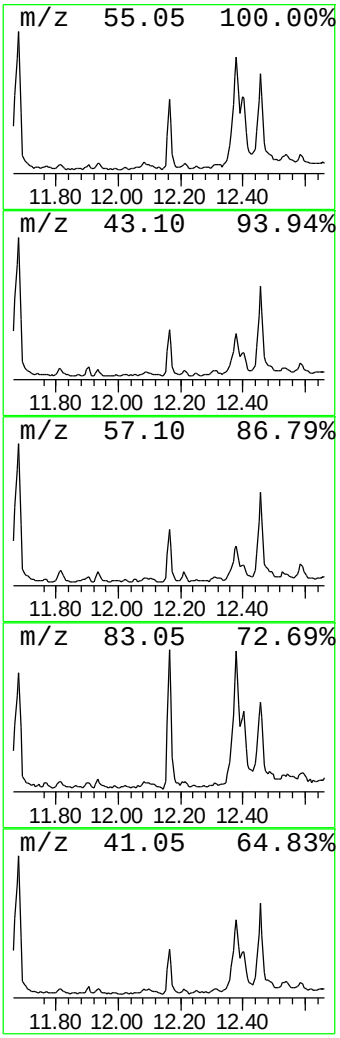
****

Peak Number 9 1-Nonadecene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	16.55 ng	445549	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Octadecene	252	C18H36	000112-88-9	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	1-Heptadecene	238	C17H34	006765-39-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

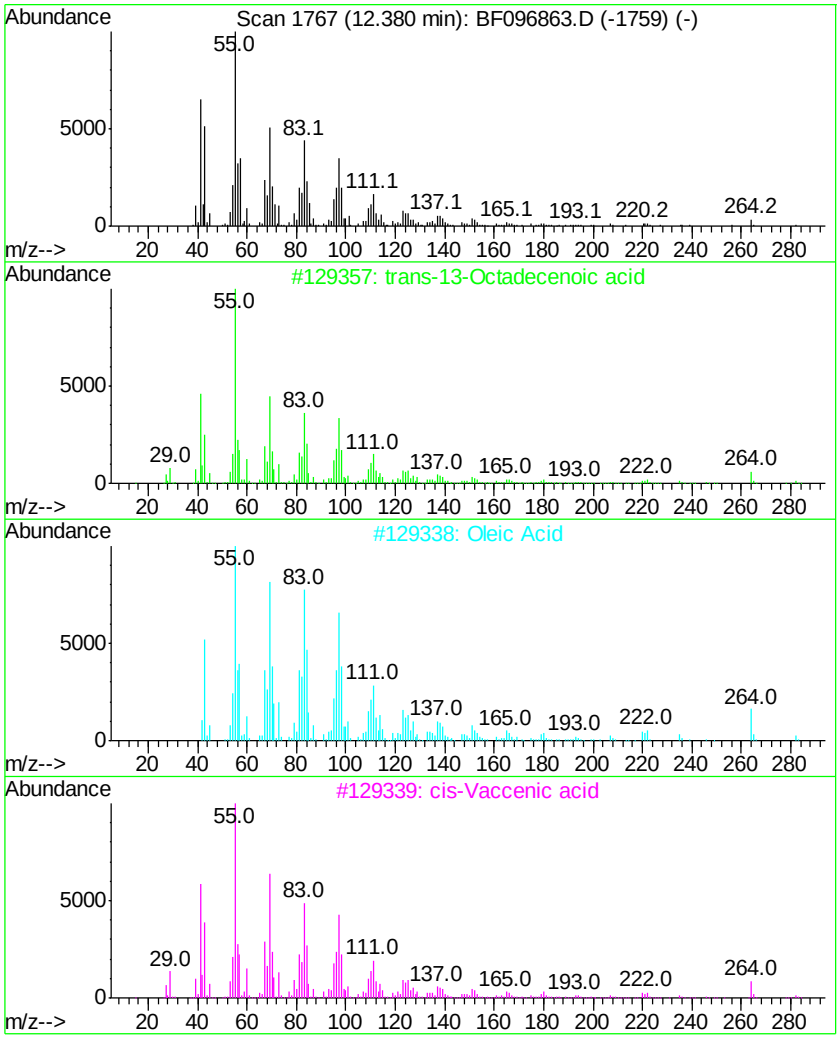
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

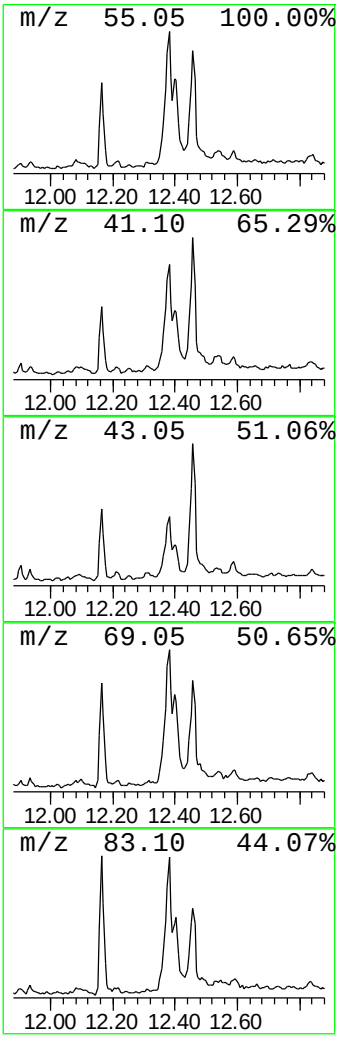
****

Peak Number 10 trans-13-Octadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	41.42 ng	1114930	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	98
2	Oleic Acid	282	C18H34O2	000112-80-1	96
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
4	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
5	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

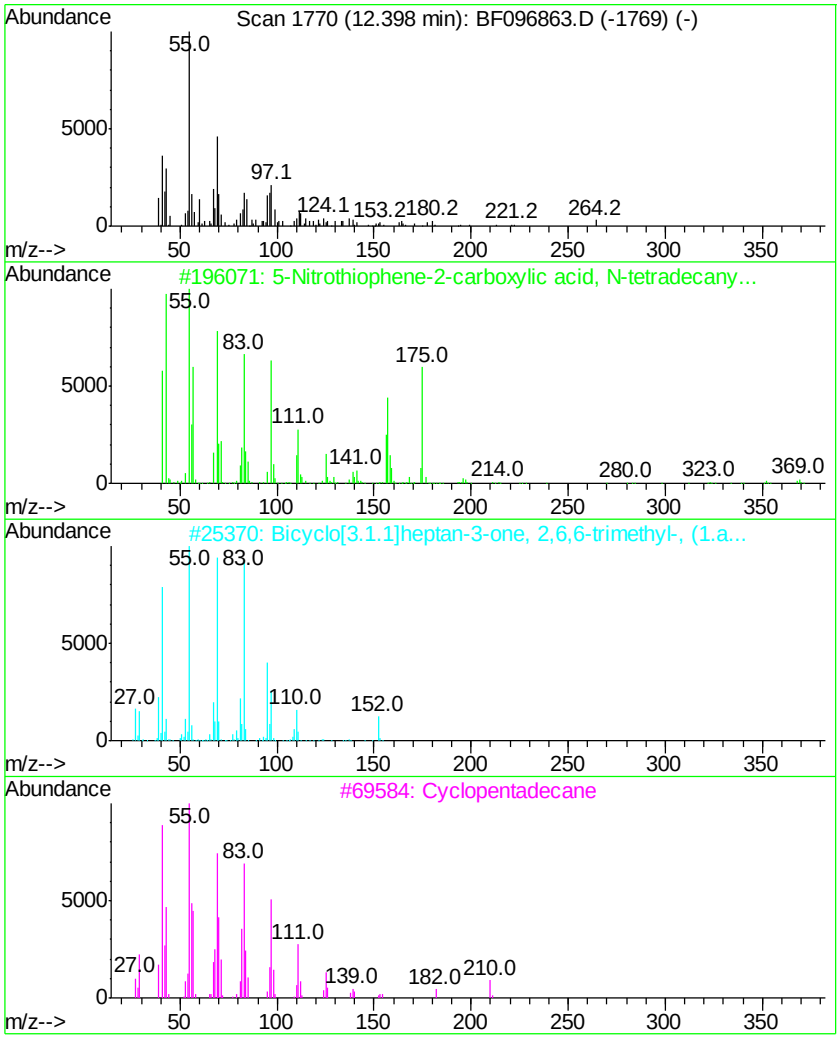
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

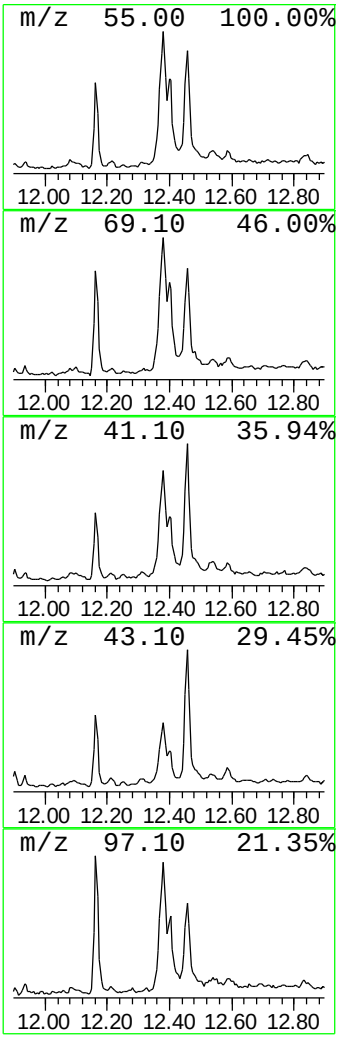
****

Peak Number 11 unknown12.40 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	17.97 ng	483803	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Nitrothiophene-2-carboxylic ac...	369	C19H31NO4S	1000253-28-2	38
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	30
3	Cyclopentadecane	210	C15H30	000295-48-7	25
4	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	22
5	Cyclohexadecane	224	C16H32	000295-65-8	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

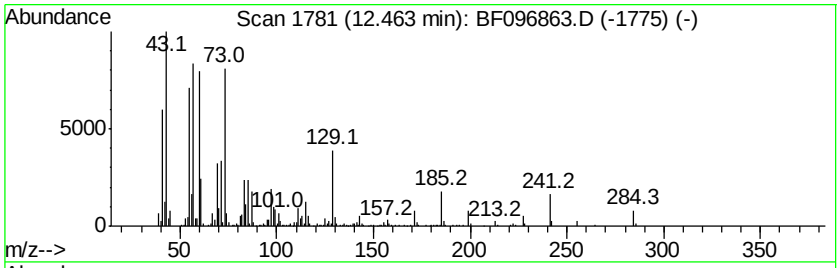
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

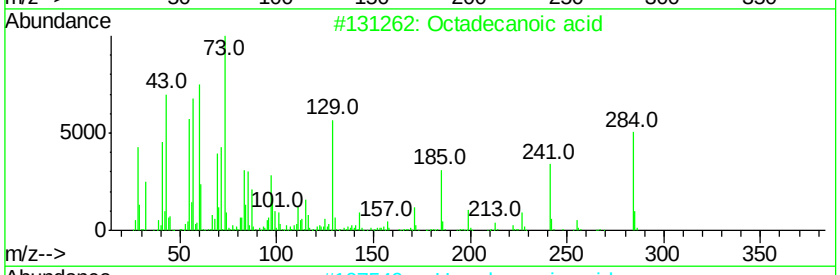
****

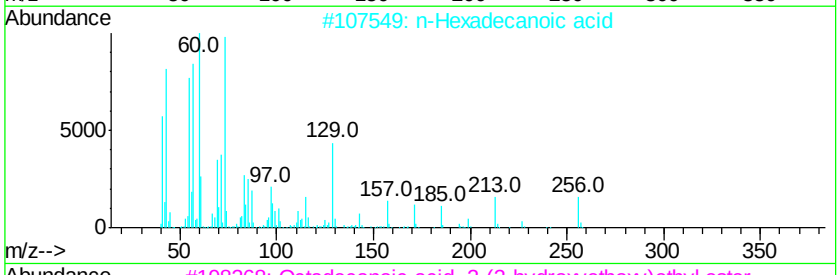
Peak Number 12 Octadecanoic acid Concentration Rank 4

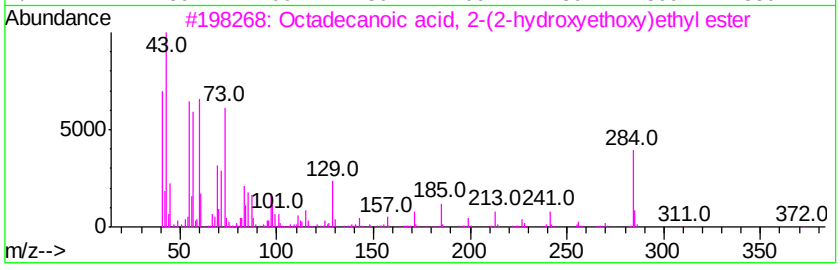
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	64.68 ng	1281650	Chrysene-d12	13.73

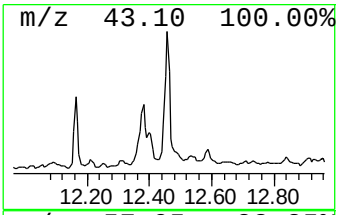
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72

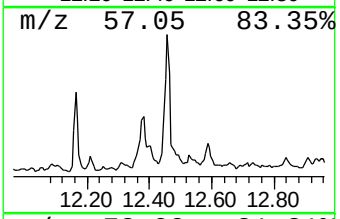


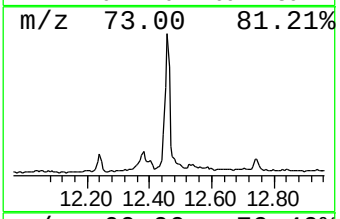


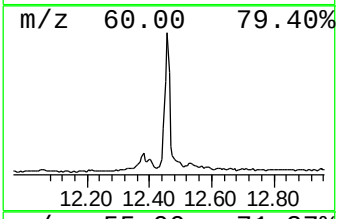


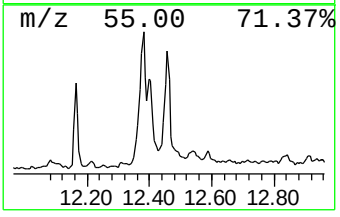












Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

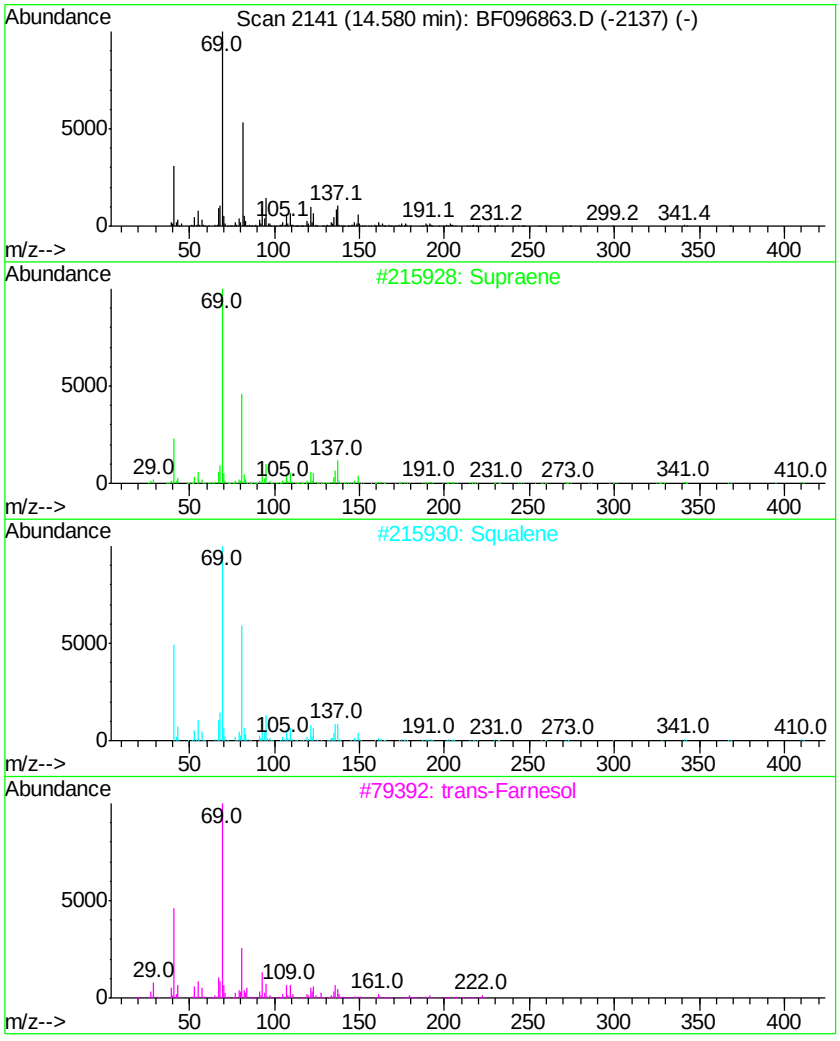
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

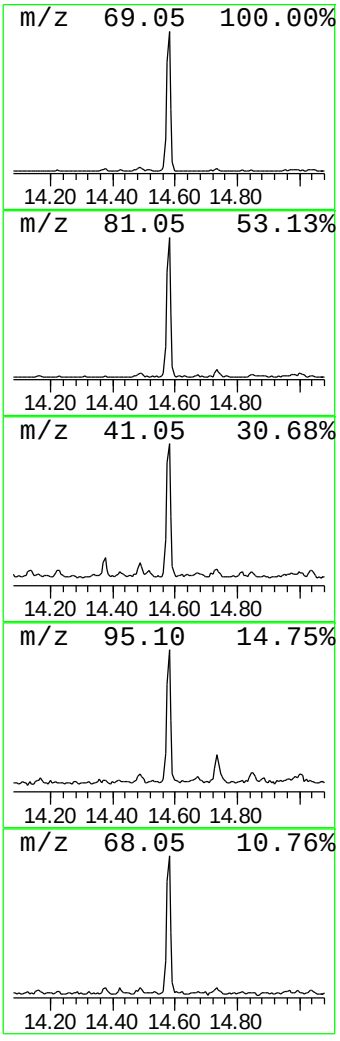
****

Peak Number 13 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	63.92 ng	861923	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	trans-Farnesol	222	C15H26O	000106-28-5	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

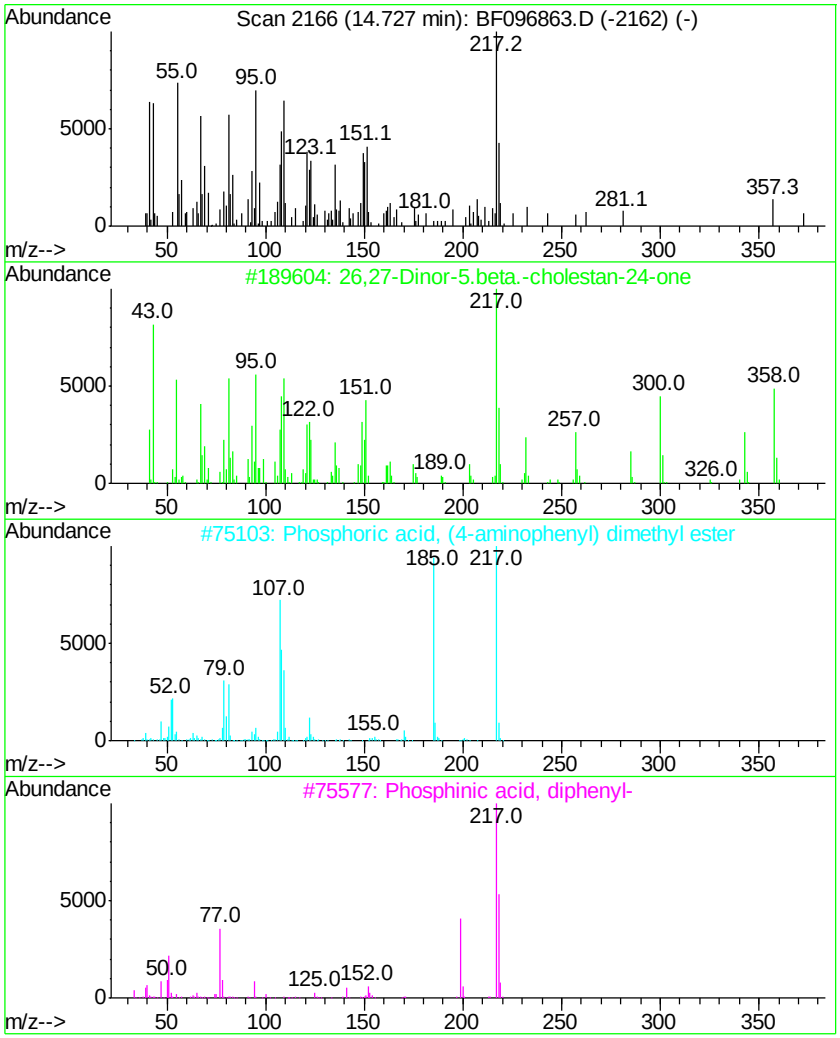
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

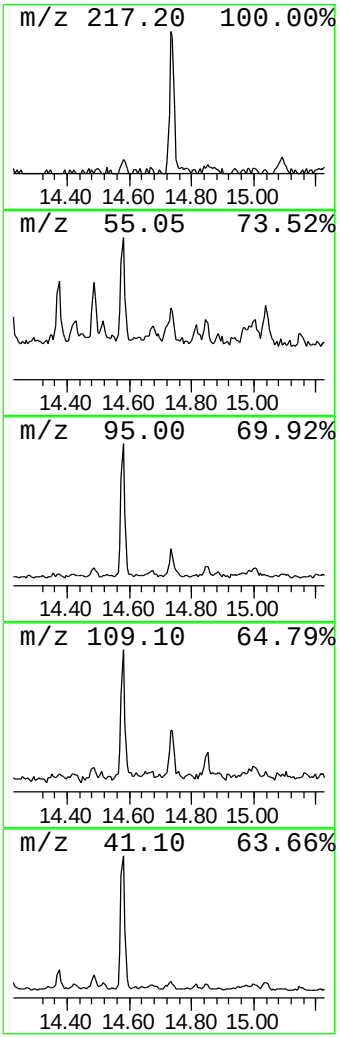
****

Peak Number 14 26,27-Dinor-5.beta.-cholest... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	15.99 ng	215548	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	26,27-Dinor-5.beta.-cholestan-24...	358	C25H42O	014949-16-7	87
2	Phosphoric acid, (4-aminophenyl)...	217	C8H12NO4P	123363-36-0	25
3	Phosphinic acid, diphenyl-	218	C12H11O2P	001707-03-5	22
4	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	14
5	Pyrimidin-2-amine, 4-methyl-6-(2...	218	C10H10N4S	283171-79-9	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

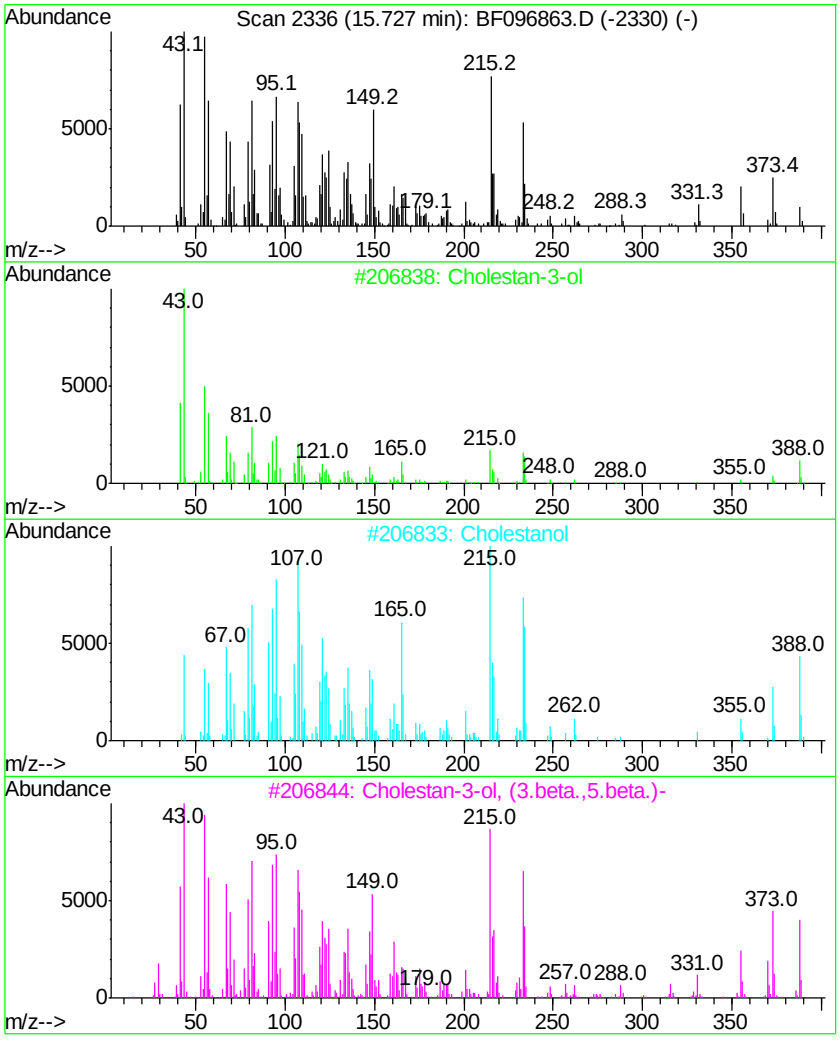
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

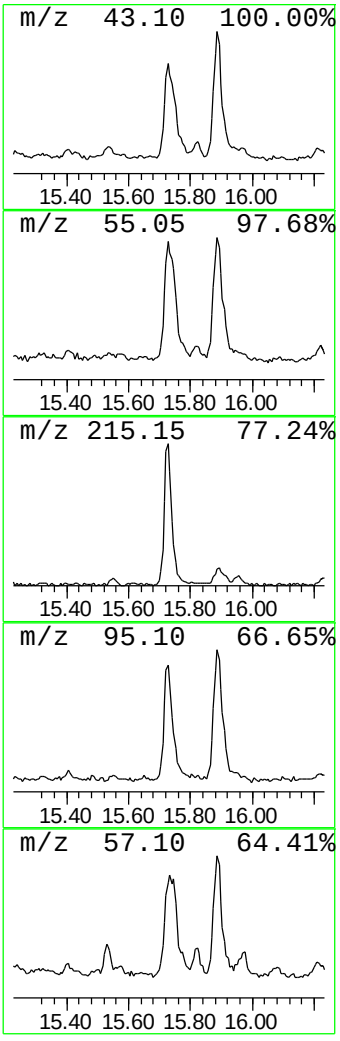
****

Peak Number 15 Cholestan-3-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	134.24 ng	1809950	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol	388	C27H48O	027409-41-2	87
2	Cholestanol	388	C27H48O	000080-97-7	58
3	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	50
4	2,3-Dichlorothiophene-5-sulfonyl...	250	C4HCl3O2S2	126714-85-0	25
5	6-Methyl-2-phenoxymethyl-4-pyrim...	215	C12H13N3O	067386-50-9	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

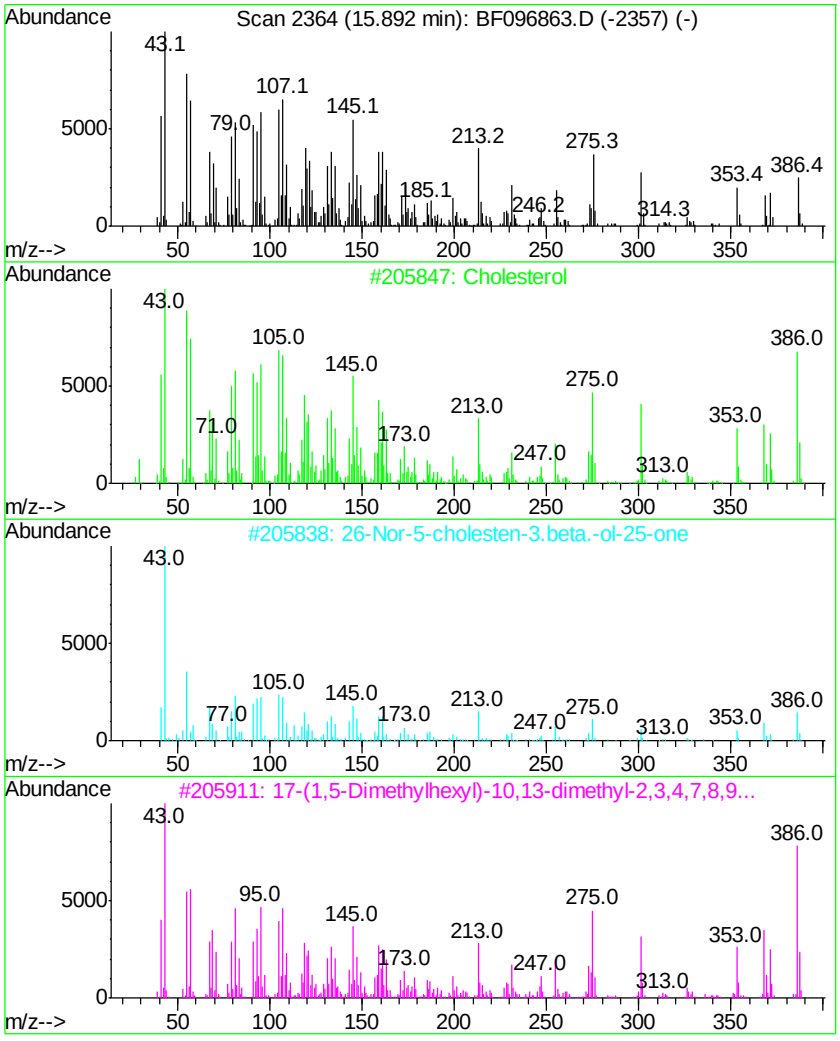
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

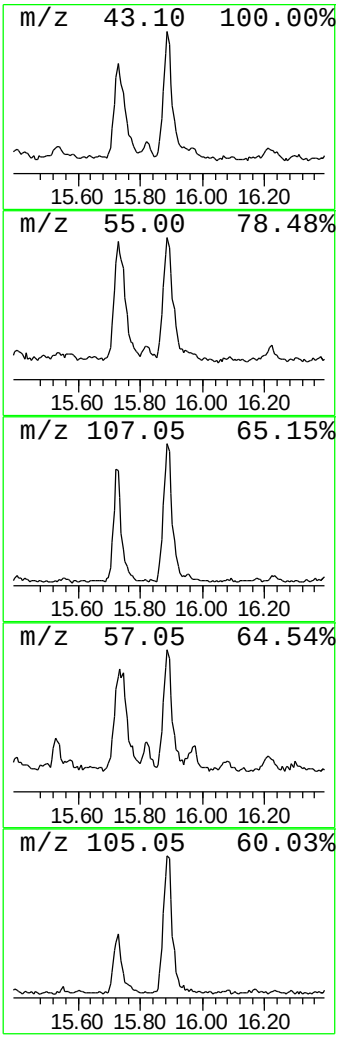
****

Peak Number 16 Cholesterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	156.98 ng	2116670	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	98
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	89
4	Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	58
5	Bicyclo[5.2.0]nonane, 4-methylen...	204	C15H24	1000159-38-2	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

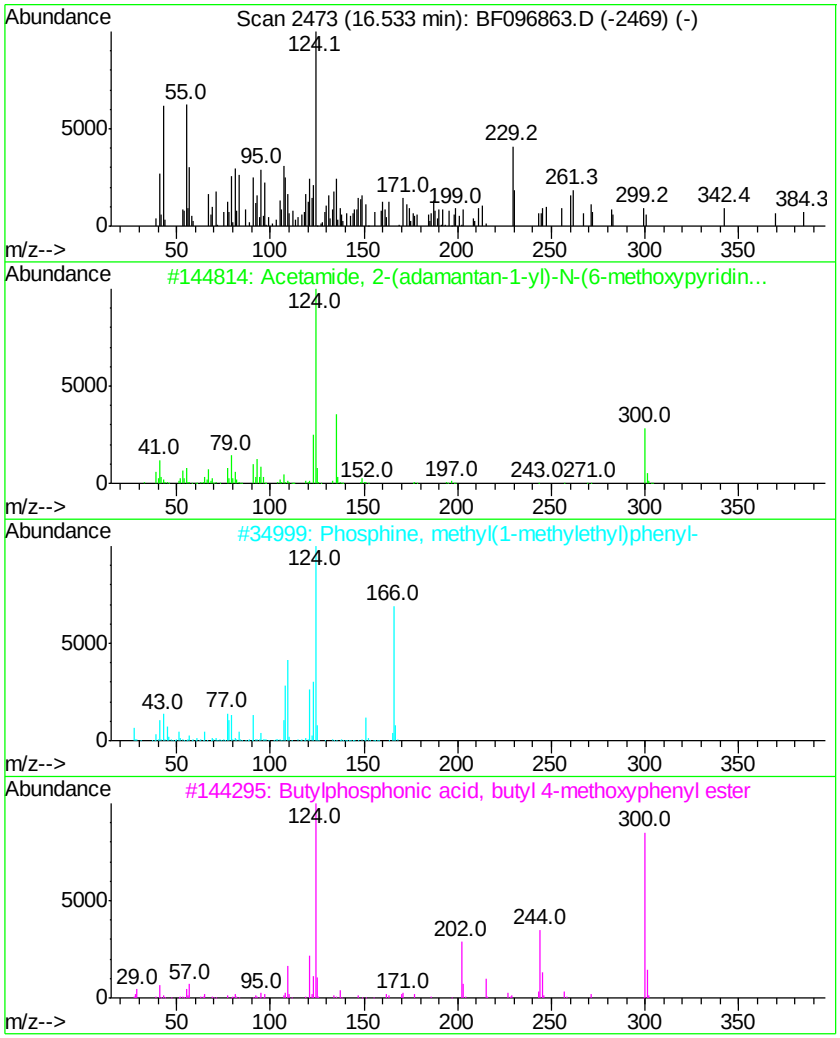
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

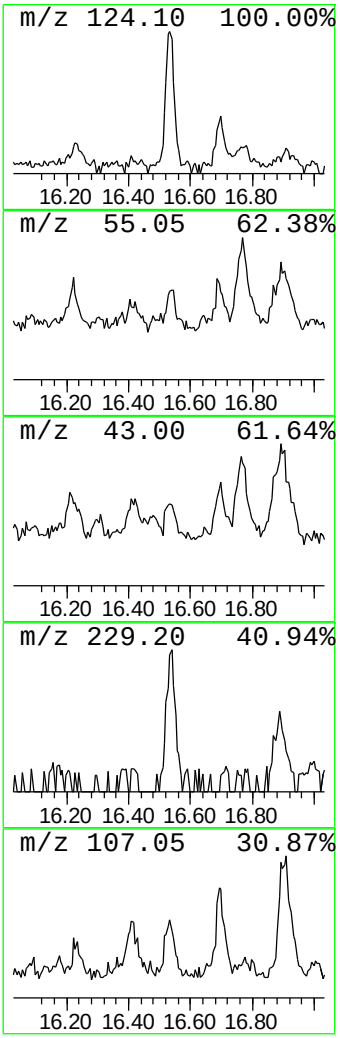
****

Peak Number 17 unknown16.53 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	15.41 ng	207821	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2-(adamantan-1-yl)-N-...	300	C18H24N2O2	1000316-15-5	38
2	Phosphine, methyl(1-methylethyl)...	166	C10H15P	036050-92-7	32
3	Butylphosphonic acid, butyl 4-me...	300	C15H25O4P	1000322-98-0	27
4	Sambucinol	266	C15H22O4	090044-33-0	25
5	Pyrimidine, 2-methoxy-5-methyl-	124	C6H8N2O	017758-07-5	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

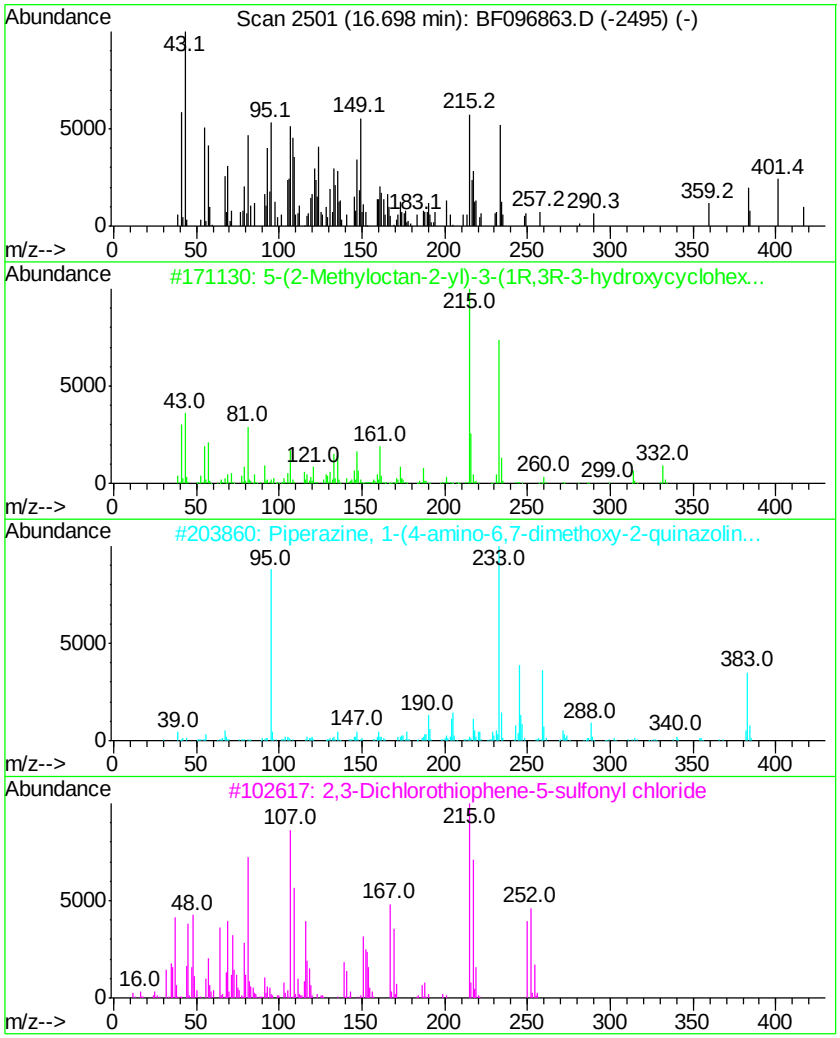
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

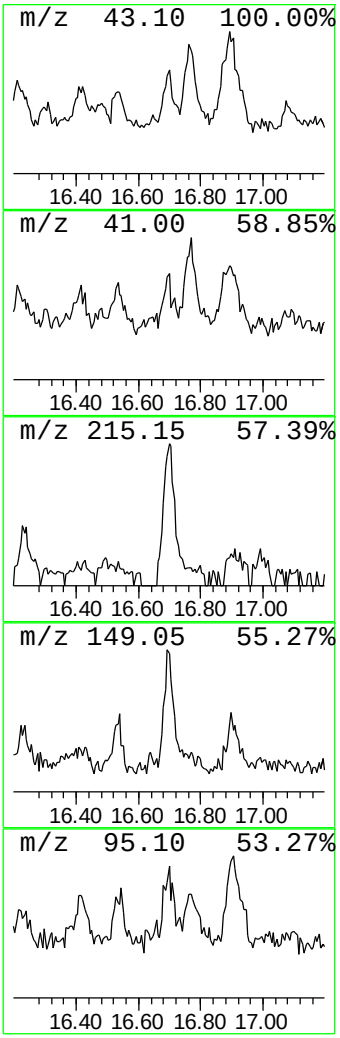
****

Peak Number 18 unknown16.70 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	15.52 ng	209244	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	22
2	Piperazine, 1-(4-amino-6,7-dimet...	383	C19H21N5O4	019216-56-9	11
3	2,3-Dichlorothiophene-5-sulfonyl...	250	C4HCl3O2S2	126714-85-0	11
4	4-Aminodiphenylsulfone	233	C12H11NO2S	007019-01-4	11
5	Terephthalic acid, monoamide, N,...	401	C26H27NO3	1000323-91-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

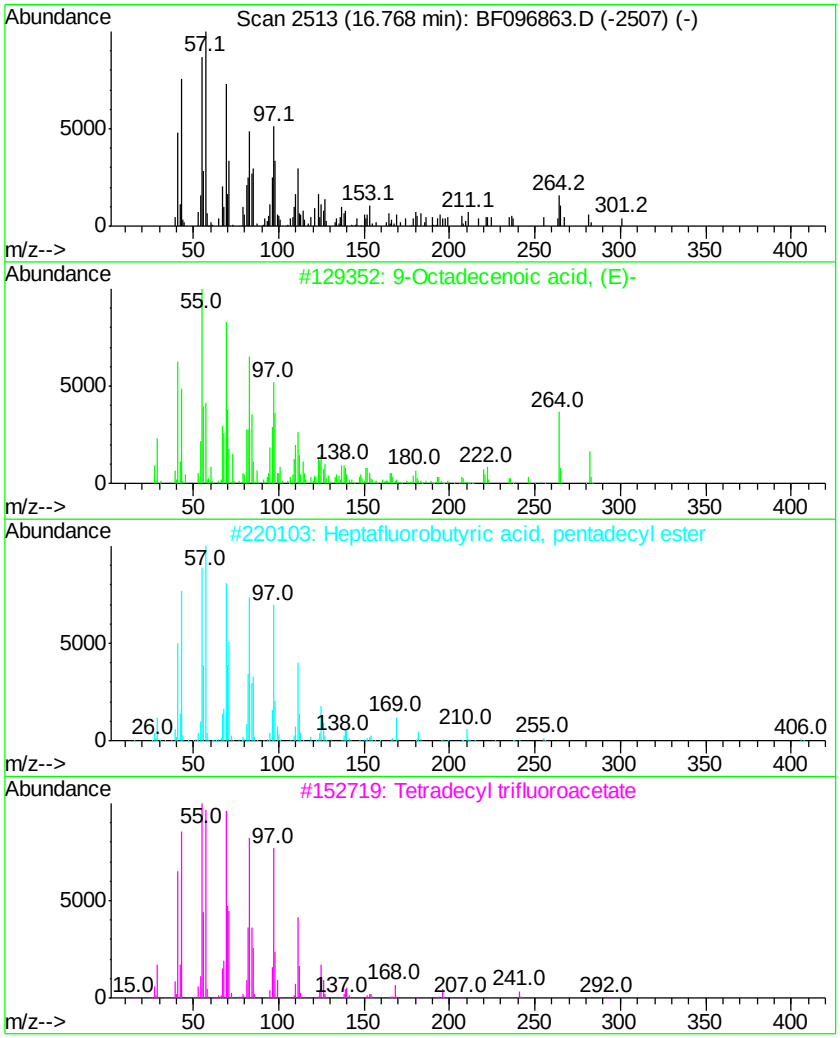
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

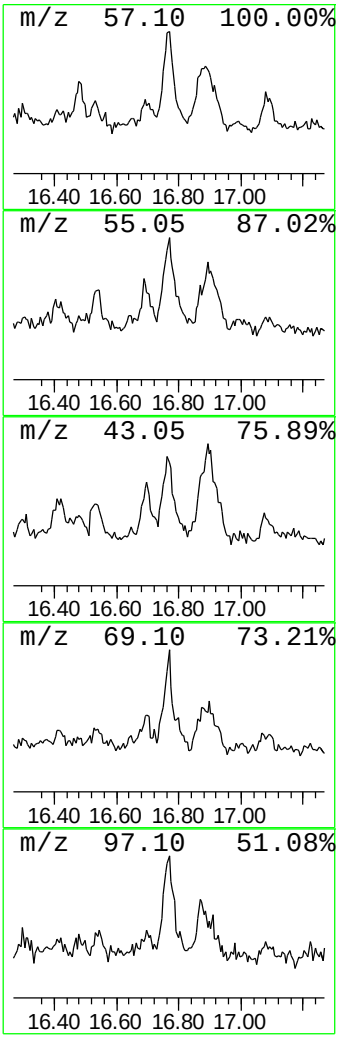
****

Peak Number 19 9-Octadecenoic acid, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	22.47 ng	302940	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	83
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	80
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	72
4	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	58
5	Decyl oleate	422	C28H54O2	003687-46-5	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

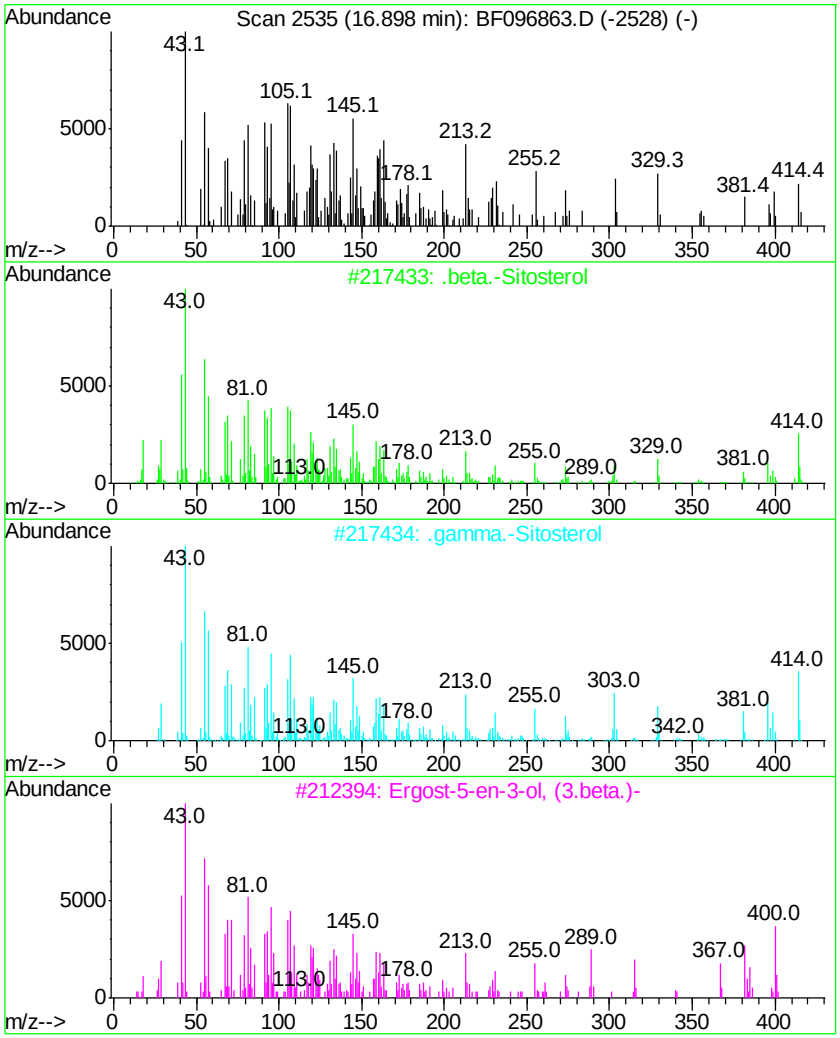
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

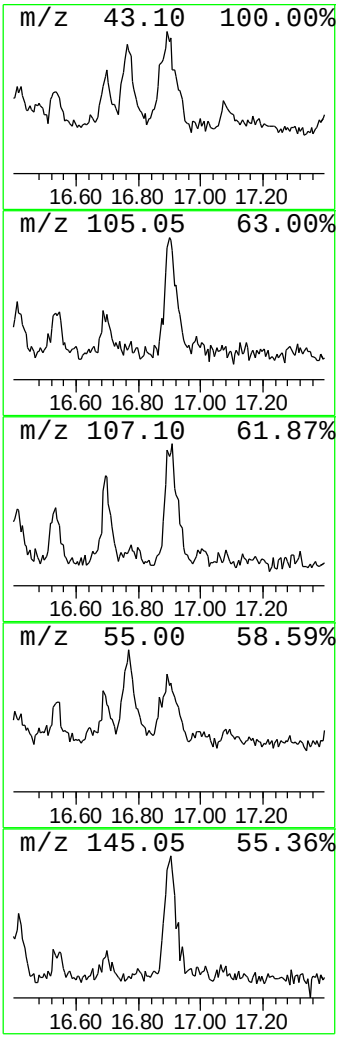
****

Peak Number 20 .beta.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	40.48 ng	545767	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	89
3	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	50
4	Campesterol	400	C28H48O	000474-62-4	50
5	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096863.D
Acq On : 19 Jul 2017 00:16
Operator : SJ/JU
Sample : I4234-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Ethylene glycol m...	5.53	21.5	ng	486451	1	6.60	452608	20.0
unknown6.37	6.37	11.9	ng	270475	1	6.60	452608	20.0
Indole	8.52	11.4	ng	343756	2	7.88	605213	20.0
1-Decene	9.45	16.6	ng	721819	3	9.63	871884	20.0
Dodecanoic acid	9.87	13.7	ng	597492	3	9.63	871884	20.0
Tetradonium Bromide	10.58	13.1	ng	352442	4	11.10	538403	20.0
1-Hexadecanol	11.35	23.1	ng	621646	4	11.10	538403	20.0
Tridecanoic acid	11.68	76.0	ng	2046640	4	11.10	538403	20.0
1-Nonadecene	12.16	16.6	ng	445549	4	11.10	538403	20.0
trans-13-Octadece...	12.38	41.4	ng	1114930	4	11.10	538403	20.0
unknown12.40	12.40	18.0	ng	483803	4	11.10	538403	20.0
Octadecanoic acid	12.46	64.7	ng	1281650	5	13.73	396301	20.0
Supraene	14.58	63.9	ng	861923	6	15.10	269668	20.0
26,27-Dinor-5.bet...	14.73	16.0	ng	215548	6	15.10	269668	20.0
Cholestan-3-ol	15.73	134.2	ng	1809950	6	15.10	269668	20.0
Cholesterol	15.89	157.0	ng	2116670	6	15.10	269668	20.0
unknown16.53	16.53	15.4	ng	207821	6	15.10	269668	20.0
unknown16.70	16.70	15.5	ng	209244	6	15.10	269668	20.0
9-Octadecenoic ac...	16.77	22.5	ng	302940	6	15.10	269668	20.0
.beta.-Sitosterol	16.90	40.5	ng	545767	6	15.10	269668	20.0