LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096971.D
Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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	4.728	463	466	474	rVB	465140	605615	3.47%	0.522%
2	4.940	483	502	504	rBV3	101035	346586	1.99%	0.299%
3	5.116	528	532	534	rBV	125480	203727	1.17%	0.175%
4	5.163	536	540	545	rBV	984233	1027989	5.90%	0.885%
5	5.498	579	597	600	rBV	201764	749666	4.30%	0.646%
6	6.216	715	719	726	rBV2	490827	827698	4.75%	0.713%
7	6.328	734	738	745	rVB	1601073	1697721	9.74%	1.462%
8	6.557	773	777	780	rBV	867667	792001	4.54%	0.682%
9	6.710	800	803	810	rVV	2112688	2047448	11.74%	1.764%
10	6.992	838	851	860	rBV2	1553987	1970451	11.30%	1.697%
11	7.122	867	873	876	rBV	1722811	1699523	9.75%	1.464%
12	7.181	880	883	886	rVV	234045	217086	1.25%	0.187%
13	7.304	902	904	908	rVV	269394	265821	1.52%	0.229%
14	7.716	953	974	977	rBV2	807114	3036511	17.42%	2.615%
15	7.763	977	982	984	rBV	432350	410215	2.35%	0.353%
16	7.839	991	995	997	rBV	1110843	961553	5.52%	0.828%
17	7.875	997	1001	1003	rVB2	380084	372387	2.14%	0.321%
18	8.010	1020	1024	1033	rVB	1641852	1619864	9.29%	1.395%
19	8.181	1042	1053	1056	rVB	794686	1548498	8.88%	1.334%
20	8.251	1061	1065	1068	rVV	271377	247437	1.42%	0.213%
21	8.445	1094	1098	1101	rVV3	227524	301794	1.73%	0.260%
22	8.486	1101	1105	1108	rVB	1428298	1143212	6.56%	0.985%
23	8.833	1154	1164	1168	rVV	1105982	2261043	12.97%	1.948%
24	8.916	1173	1178	1181	rVV	2783958	2613004	14.99%	2.251%
25	9.316	1242	1246	1252	rBV4	232335	380927	2.19%	0.328%
26	9.416	1257	1263	1266	rBV	3522966	3250055	18.64%	2.799%
27	9.586	1288	1292	1293	rBV	900009	870272	4.99%	0.750%
28	9.604	1293	1295	1300	rVV	1246104	1504861	8.63%	1.296%
29	9.645	1300	1302	1307	rVB2	212649	363209	2.08%	0.313%
30	9.886	1327	1343	1345	rBV	2487108	6112429	35.06%	5.265%
31	9.928	1347	1350	1352	rVV	568883	485991	2.79%	0.419%
32	9.980	1356	1359	1361	rVV	897579	832391	4.77%	0.717%
33	10.010	1361	1364	1367	rVB	250169	211632	1.21%	0.182%
34	10.304	1411	1414	1420	rVB3	374102	362988	2.08%	0.313%

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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

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Peak separation: 5

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

35	10.375	1422	1426	1428	rBV	811215	778255	4.46%	0.670%
36	10.410	1429	1432	1436	rVB	1531442	1314079	7.54%	1.132%
37	10.557	1453	1457	1461	rVV	1149816	1704759	9.78%	1.468%
38	10.598	1461	1464	1469	rVB	1468550	1472366	8.45%	1.268%
39	10.798	1489	1498	1505	rVV	2347396	4526184	25.96%	3.899%
40	10.869	1508	1510	1516	rVB	446968	407362	2.34%	0.351%
41	11.057	1535	1542	1545	rBV2	875726	1091182	6.26%	0.940%
42	11.086	1545	1547	1550	rVB	238744	177847	1.02%	0.153%
43	11.145	1554	1557	1560	rVB	544748	472287	2.71%	0.407%
44	11.210	1564	1568	1571	rBV2	580476	525262	3.01%	0.452%
45	11.251	1571	1575	1578	rVB2	434025	401610	2.30%	0.346%
46	11.310	1581	1585	1588	rBV	745483	689081	3.95%	0.594%
47	11.427	1600	1605	1606	rBV2	256882	260489	1.49%	0.224%
48	11.451	1606	1609	1612	rVV	352049	559618	3.21%	0.482%
49	11.480	1612	1614	1619	rVB	568394	552389	3.17%	0.476%
50	11.698	1633	1651	1654	rBV	4865897	17433663	100.00%	15.016%
51	11.780	1662	1665	1669	rBV	1221547	1020596	5.85%	0.879%
52	12.027	1704	1707	1720	rVB4	413220	594997	3.41%	0.512%
53	12.127	1720	1724	1729	rBV	1165915	1084947	6.22%	0.935%
54	12.174	1729	1732	1734	rBV	215265	191543	1.10%	0.165%
55	12.239	1740	1743	1746	rBV	184239	204250	1.17%	0.176%
56	12.369	1753	1765	1770	rBV3	1827529	5569820	31.95%	4.797%
57	12.439	1771	1777	1780	rVB	2718754	3950361	22.66%	3.403%
58	12.557	1794	1797	1799	rBV	480119	426174	2.44%	0.367%
59	12.651	1809	1813	1816	rVB	1446523	1456586	8.36%	1.255%
60	12.704	1820	1822	1828	rVB	171082	178438	1.02%	0.154%
61	12.804	1836	1839	1843	rBV	1449210	1363067	7.82%	1.174%
62	12.916	1856	1858	1865	rVB4	199403	283151	1.62%	0.244%
63	12.968	1865	1867	1870	rBV	176049	181068	1.04%	0.156%
64	13.139	1892	1896	1897	rBV	621605	618853	3.55%	0.533%
65	13.239	1909	1913	1915	rBV3	182276	269315	1.54%	0.232%
66	13.327	1925	1928	1931	rVB	203673	234203	1.34%	0.202%
67	13.386	1935	1938	1941	rBV3	106394	176222	1.01%	0.152%
68	13.492	1954	1956	1960	rVB	482334	421920	2.42%	0.363%
69	13.563	1965	1968	1972	rVB	336191	373073	2.14%	0.321%
70	13.616	1974	1977	1981	rVB2	170616	209738	1.20%	0.181%
71	13.692	1987	1990	1992	rVV	706458	752902	4.32%	0.648%

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Sample : I4274-04
Misc :
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Instrument : BNA_F
ClientSampleId : M-COMB-05

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

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

72	13.715	1992	1994	1998	rVB	1732166	1691179	9.70%	1.457%
73	13.815	2009	2011	2014	rVB	207217	185053	1.06%	0.159%
74	14.033	2044	2048	2051	rBV2	310070	370212	2.12%	0.319%
75	14.098	2056	2059	2063	rBV	369616	364739	2.09%	0.314%
76	14.180	2071	2073	2079	rBV	179275	211352	1.21%	0.182%
77	14.333	2096	2099	2105	rBV	869520	1007612	5.78%	0.868%
78	14.386	2105	2108	2111	rVV	358411	404052	2.32%	0.348%
79	14.451	2114	2119	2121	rBV	261710	310610	1.78%	0.268%
80	14.480	2122	2124	2128	rVV2	272464	285664	1.64%	0.246%
81	14.545	2130	2135	2143	rVV	3413151	4256610	24.42%	3.666%
82	14.627	2146	2149	2153	rVB2	281985	358337	2.06%	0.309%
83	14.674	2153	2157	2160	rBV2	226668	277917	1.59%	0.239%
84	14.839	2182	2185	2189	rBV2	162744	211914	1.22%	0.183%
85	14.951	2201	2204	2208	rVB4	339825	415329	2.38%	0.358%
86	14.992	2208	2211	2217	rVB	682458	835110	4.79%	0.719%
87	15.051	2218	2221	2227	rVB	483550	576501	3.31%	0.497%
88	15.192	2241	2245	2252	rVB	203464	322580	1.85%	0.278%
89	15.351	2269	2272	2277	rVB	172654	259140	1.49%	0.223%
90	15.451	2283	2289	2294	rBV	548264	980602	5.62%	0.845%
91	15.680	2318	2328	2337	rBV4	1042619	3455010	19.82%	2.976%
92	15.751	2338	2340	2346	rVV3	318570	605578	3.47%	0.522%
93	15.821	2347	2352	2359	rVB2	968003	1640611	9.41%	1.413%
94	16.139	2401	2406	2413	rVB2	165383	320243	1.84%	0.276%
95	16.604	2482	2485	2491	rBV6	86583	186788	1.07%	0.161%
96	16.674	2491	2497	2510	rVV	403451	1039832	5.96%	0.896%
97	16.786	2510	2516	2522	rBV3	338935	777181	4.46%	0.669%
98	18.068	2727	2734	2744	rVB4	270954	786964	4.51%	0.678%
99	18.215	2754	2759	2772	rVB2	236539	693160	3.98%	0.597%

Sum of corrected areas: 116099142

LSC Report - Integrated Chromatogram

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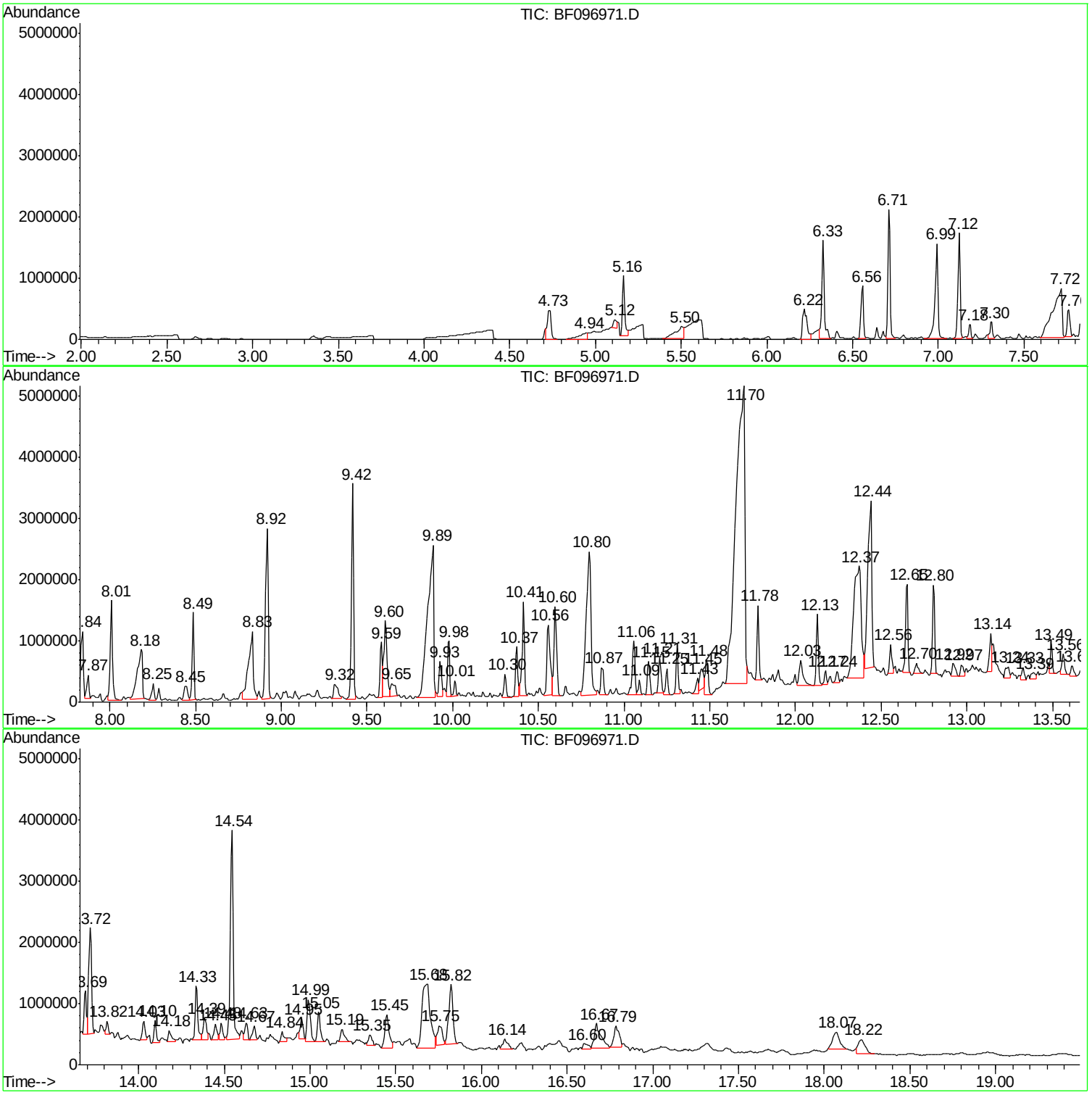
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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



Library Search Compound Report

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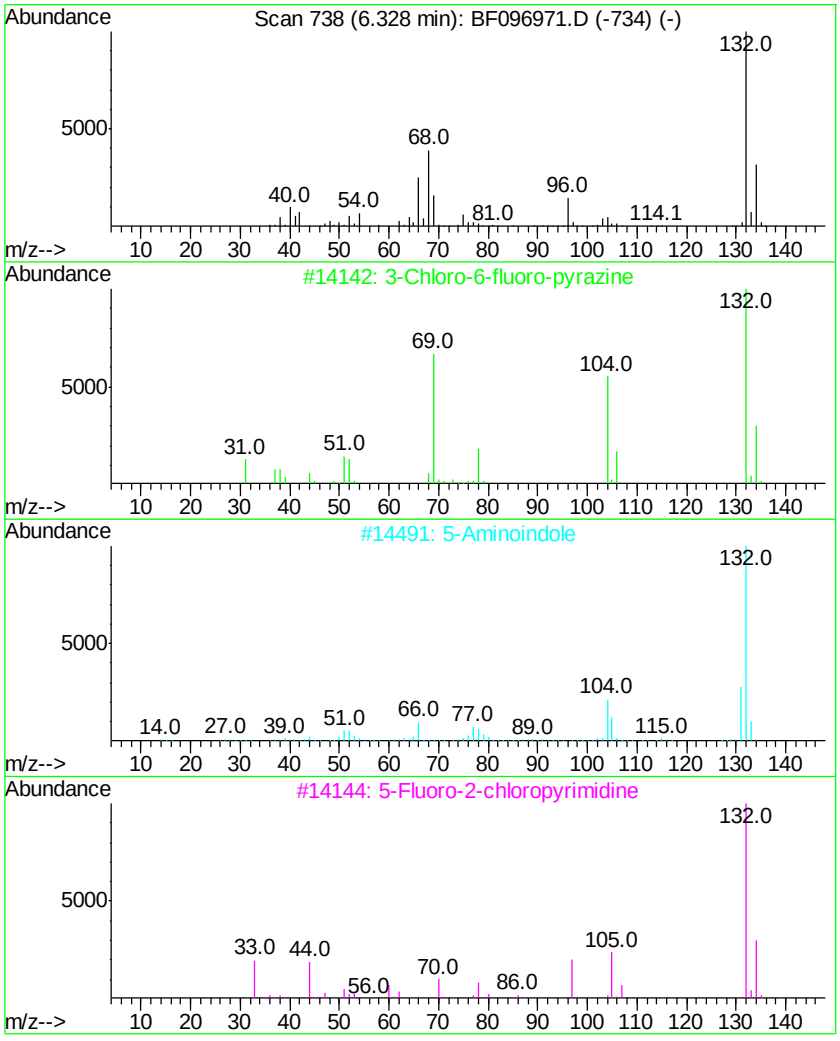
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

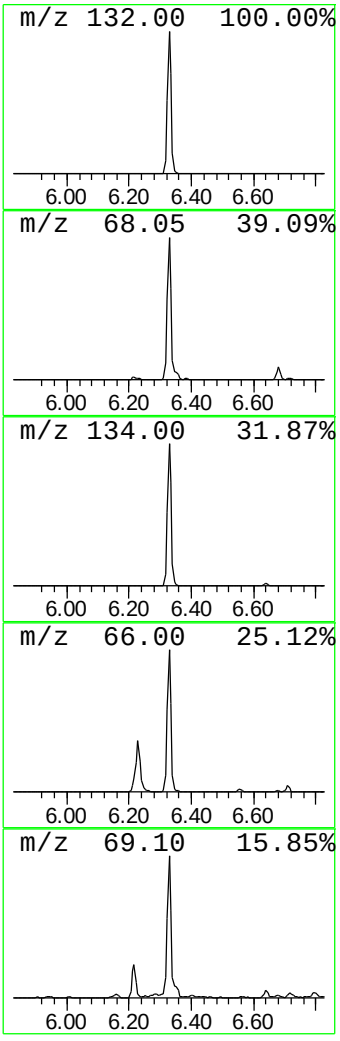
****

Peak Number 1 unknown6.33 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	42.87 ng	1697720	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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ClientSampleId : M-COMB-05

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
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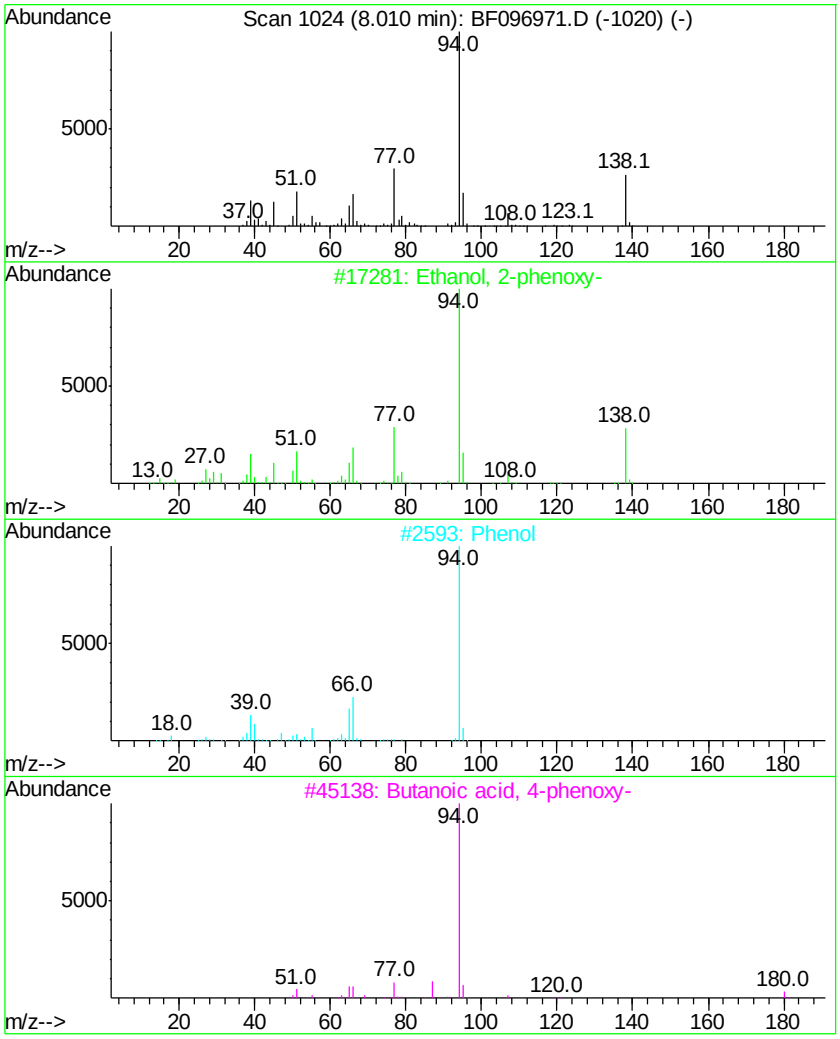
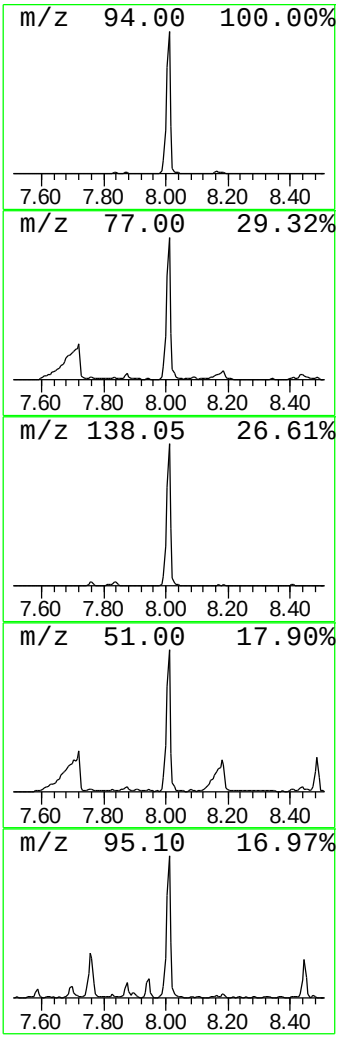
****

Peak Number 2 Ethanol, 2-phenoxy- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	33.69 ng	1619860	Naphthalene-d8	7.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	96
2	Phenol	94	C6H6O	000108-95-2	53
3	Butanoic acid, 4-phenoxy-	180	C10H12O3	006303-58-8	50
4	Carbamic acid, phenyl ester	137	C7H7NO2	000622-46-8	47
5	Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	47





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TIC Library : C:\DATABASE\NIST11.L
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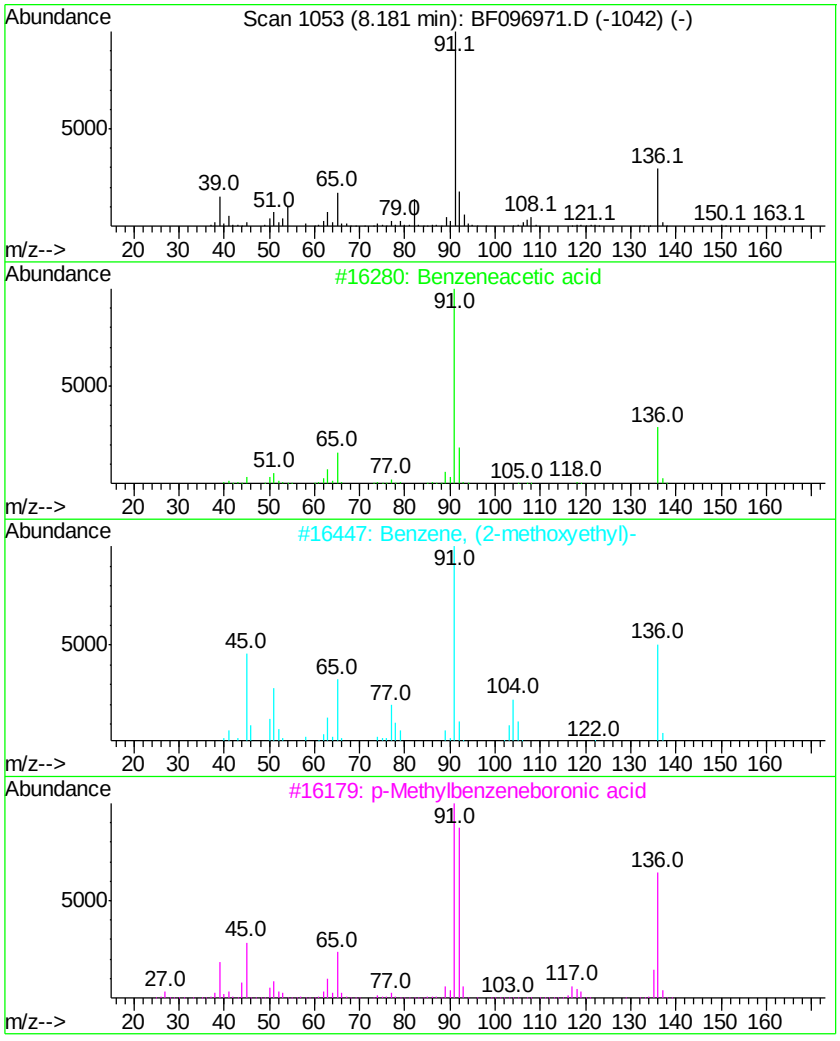
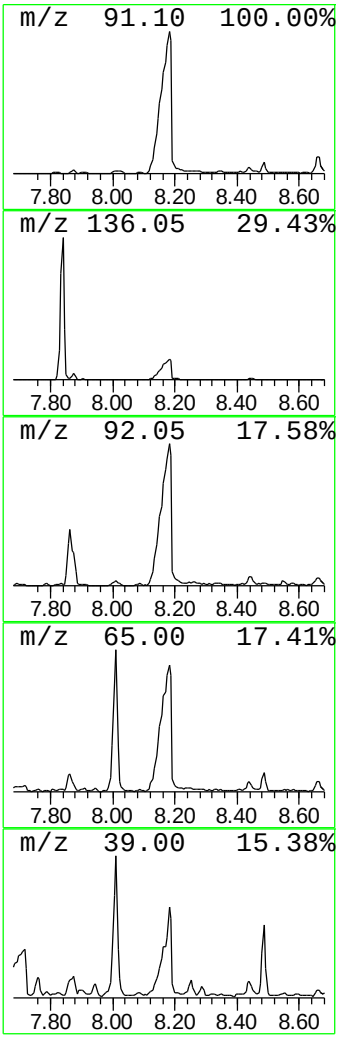
Peak Number 3 Benzeneacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	32.21 ng	1548500	Naphthalene-d8	7.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	92
2	Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	50
3	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	47
4	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	43
5	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	38





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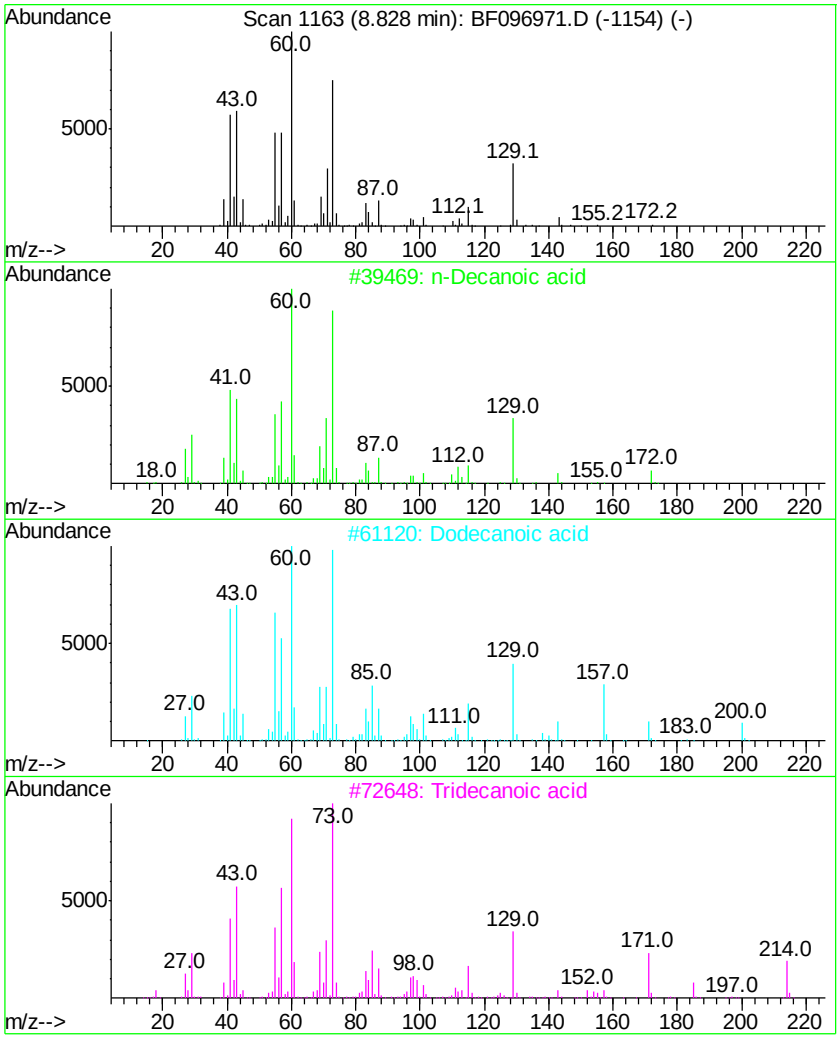
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

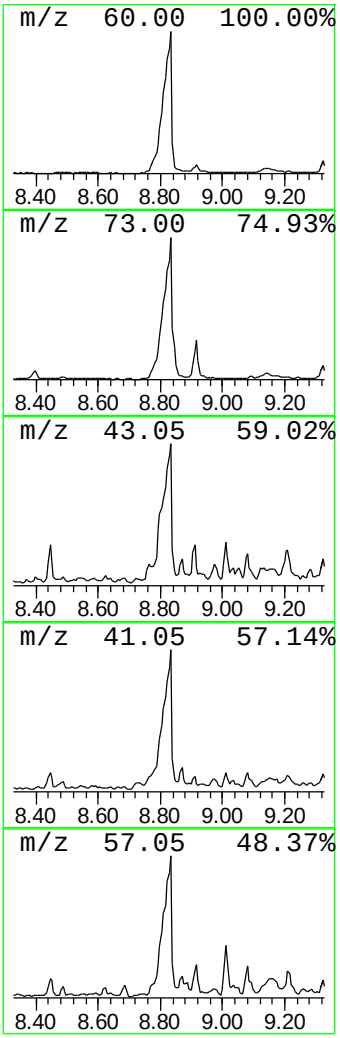
****

Peak Number 4 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	51.96 ng	2261040	Acenaphthene-d10	9.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	90
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	53
5	Hexanoic acid	116	C6H12O2	000142-62-1	52





Library Search Compound Report

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Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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

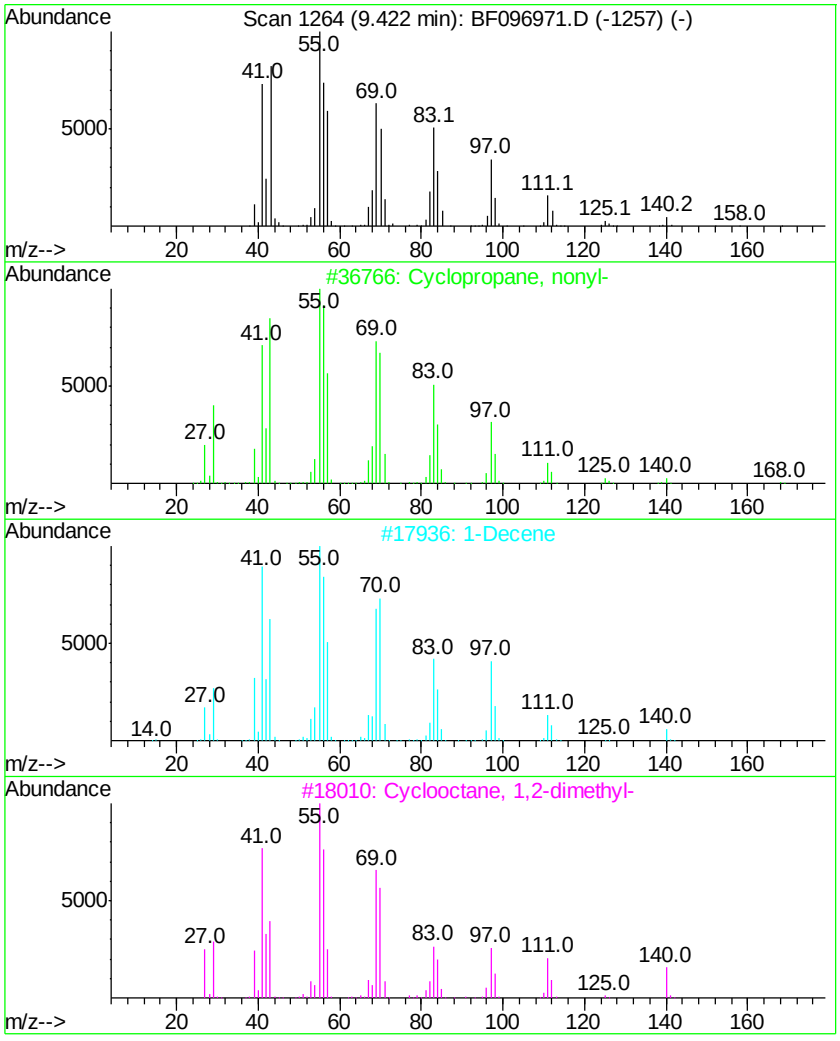
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

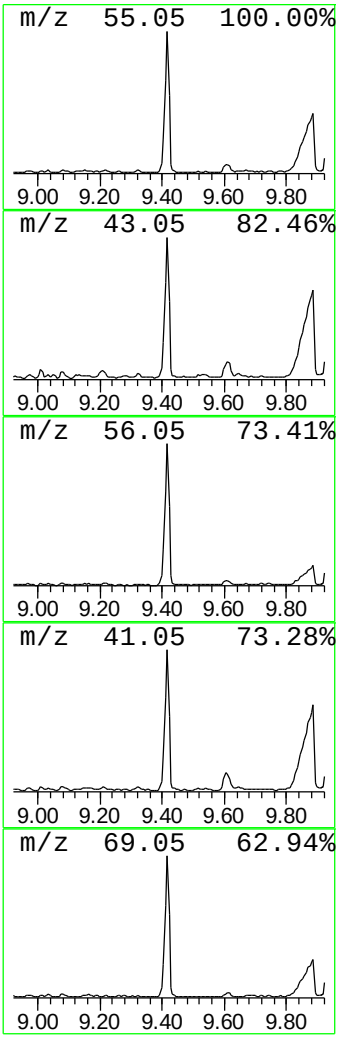
****

Peak Number 5 Cyclopropane, nonyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	74.69 ng	3250060	Acenaphthene-d10	9.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, nonyl-	168	C12H24	074663-85-7	96
2	1-Decene	140	C10H20	000872-05-9	94
3	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	93
4	1-Dodecanol	186	C12H26O	000112-53-8	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	90





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Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

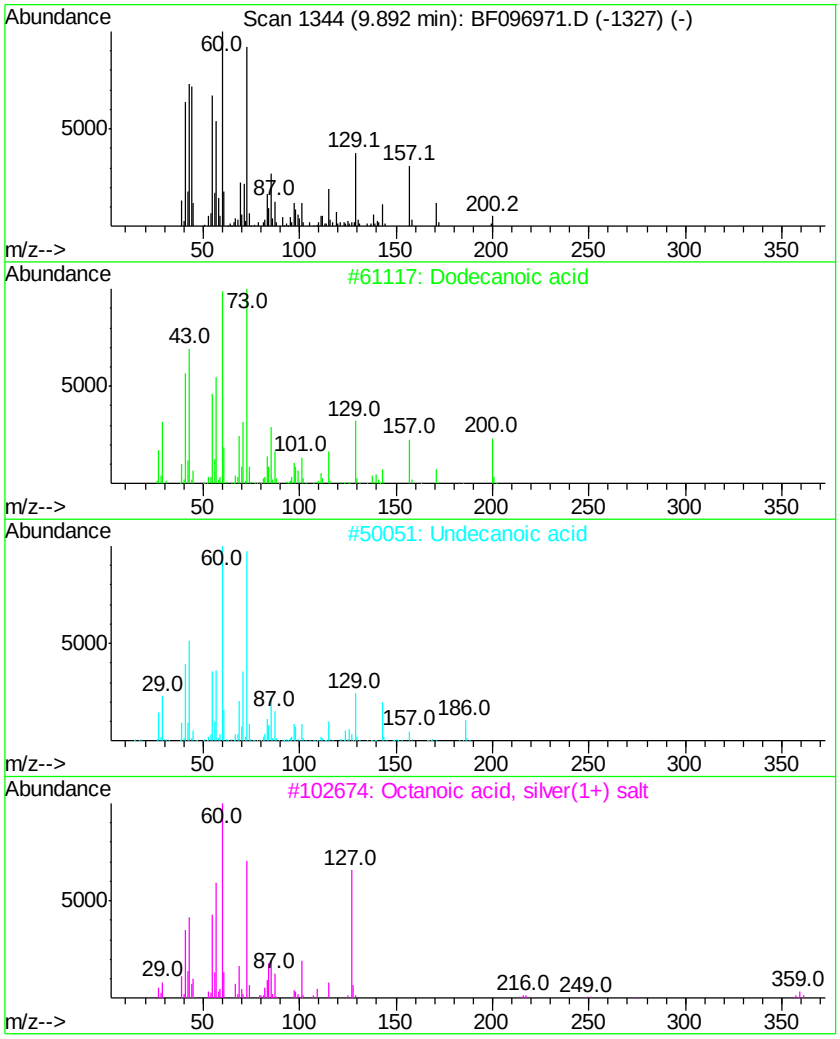
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

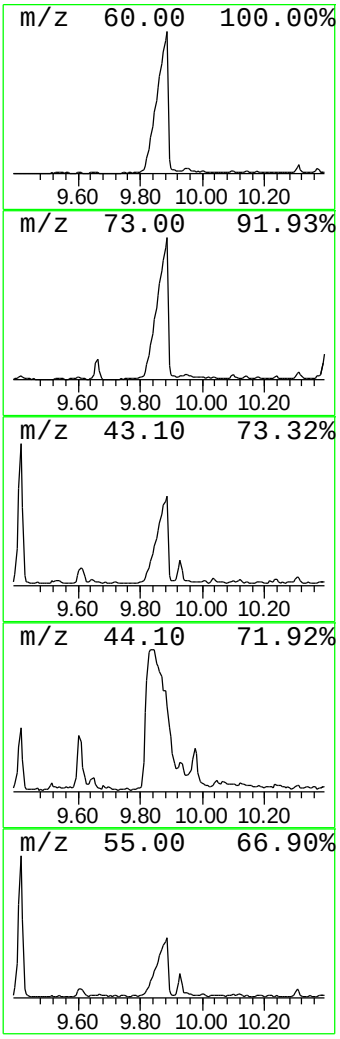
****

Peak Number 6 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.89	140.47 ng	6112430	Acenaphthene-d10	9.59

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	80
3	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	53
4	Octanoic acid	144	C8H16O2	000124-07-2	50
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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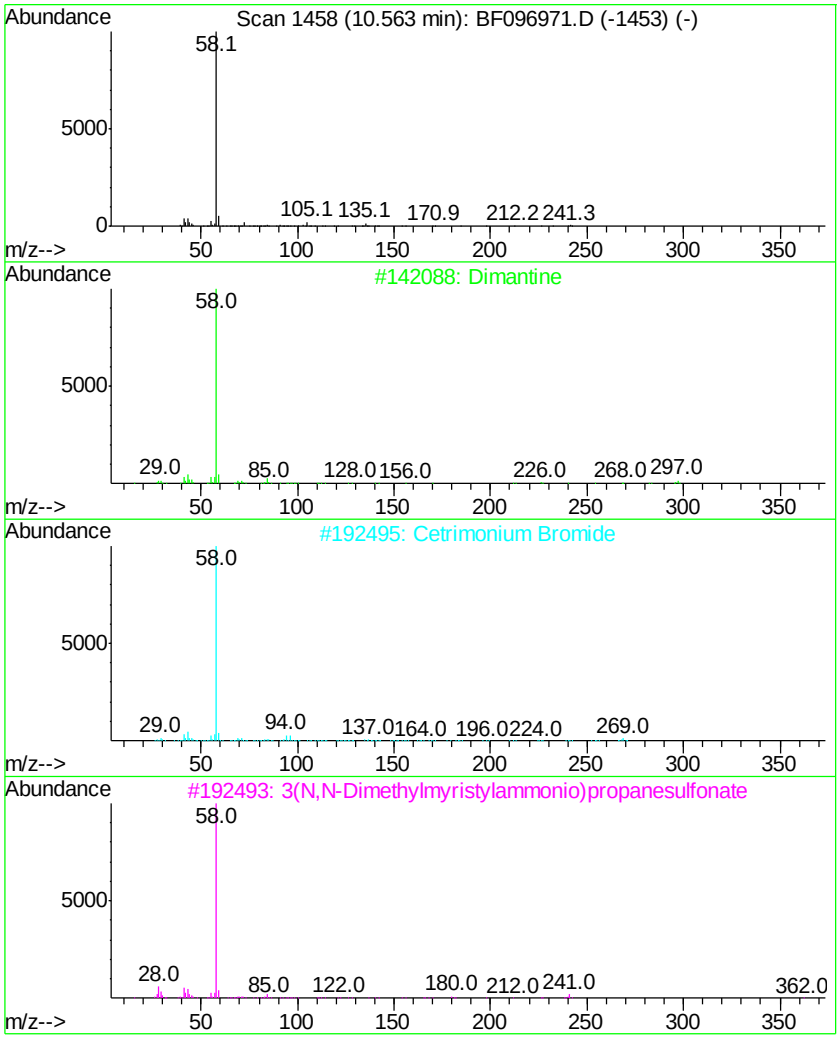
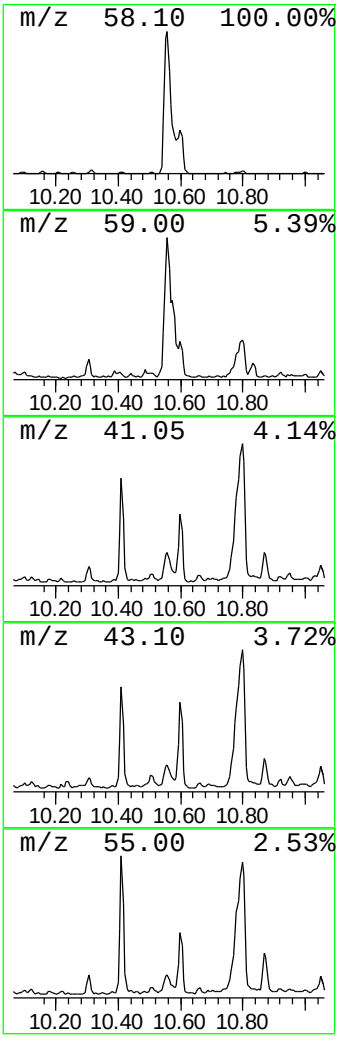
Peak Number 7 Dimantine Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	31.25 ng	1704760	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimantine	297	C20H43N	000124-28-7	72
2	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	72
3	3(N,N-Dimethylmyristylammonio)pr...	363	C19H41NO3S	014933-09-6	72
4	1-Pentadecanamine, N,N-dimethyl-	255	C17H37N	017678-60-3	72
5	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72





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Instrument : BNA_F
ClientSampleId : M-COMB-05

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TIC Integration Parameters: LSCINT.P

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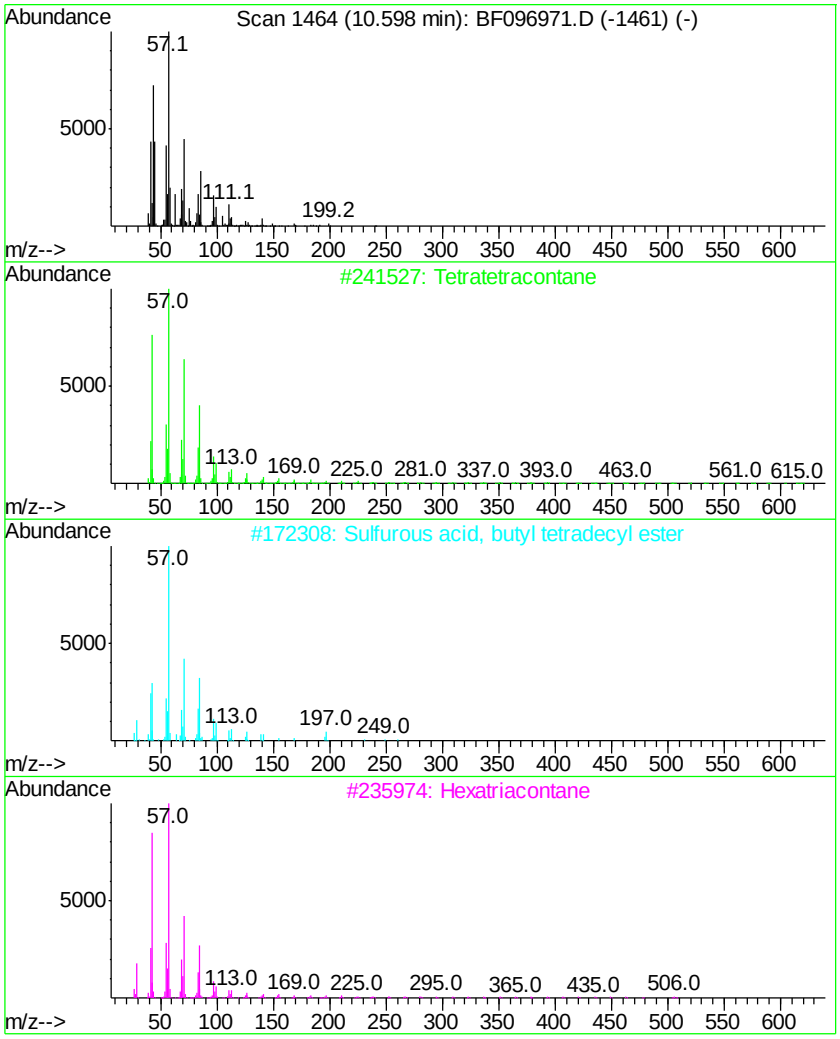
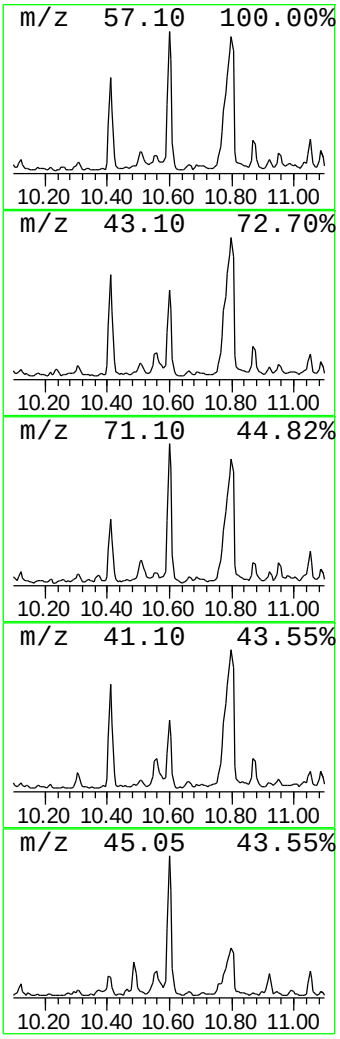
Peak Number 8 unknown10.60 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	26.99 ng	1472370	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	49
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	49
3	Hexatriacontane	507	C36H74	000630-06-8	49
4	Tritetracontane	605	C43H88	007098-21-7	49
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	46





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ClientSampleId : M-COMB-05

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

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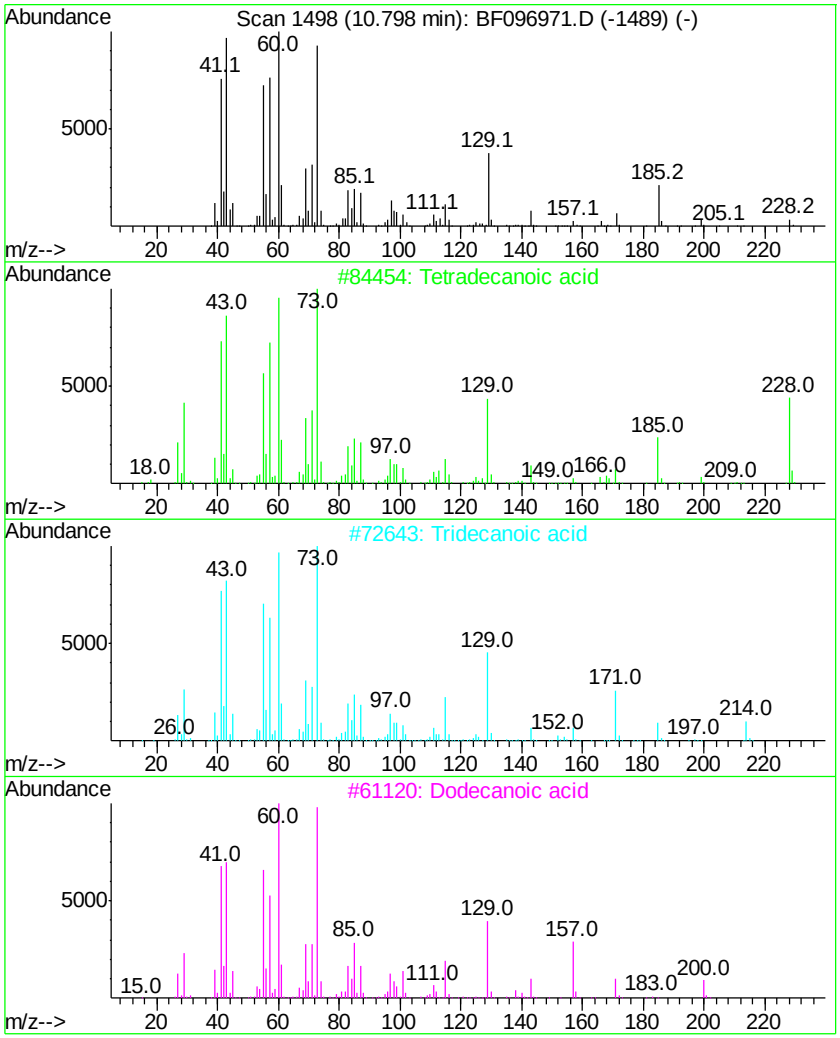
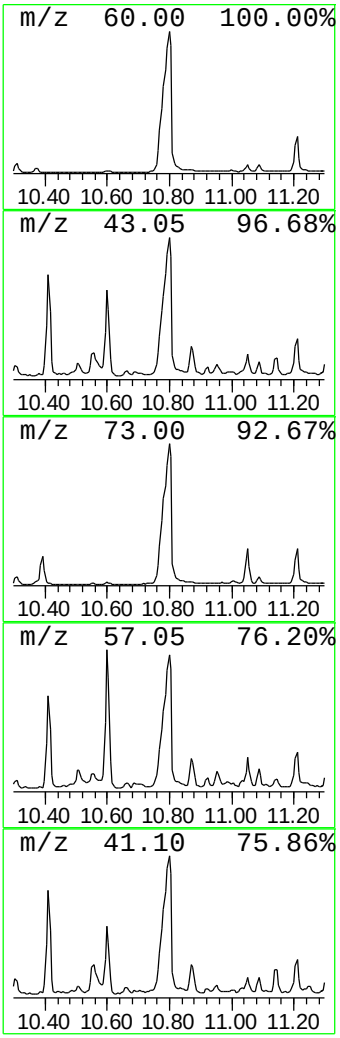
Peak Number 9 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	82.96 ng	4526180	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	59
5	Acetamide, N-(2-hydroxyethyl)-	103	C4H9NO2	000142-26-7	35





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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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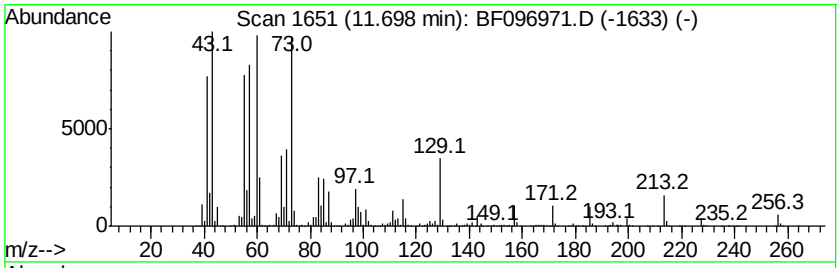
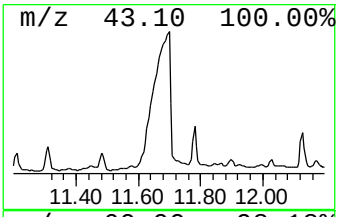
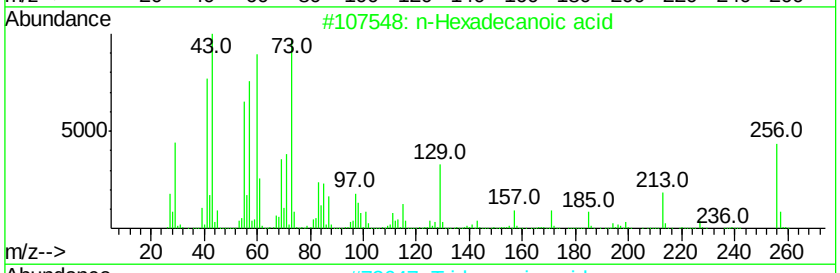
Peak Number 10 n-Hexadecanoic acid Concentration Rank 1

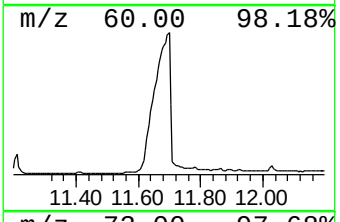
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	319.54 ng	17433700	Phenanthrene-d10	11.06

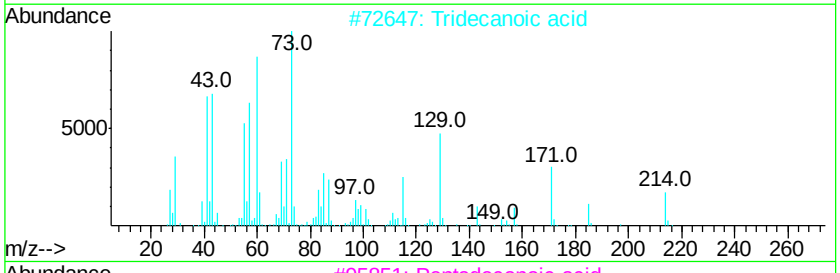
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

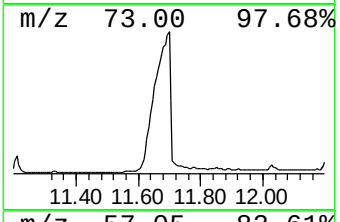


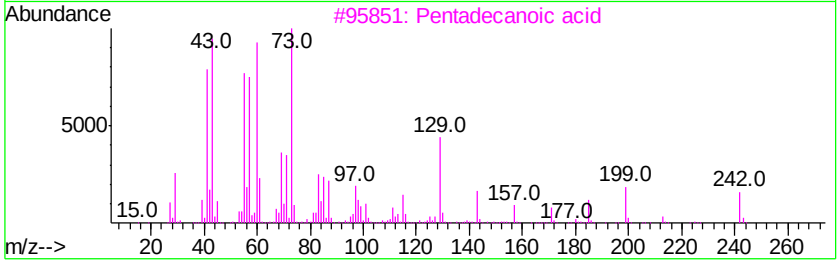


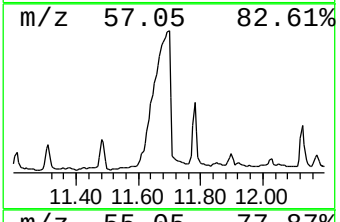


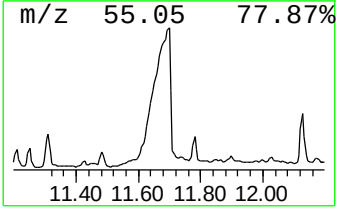












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Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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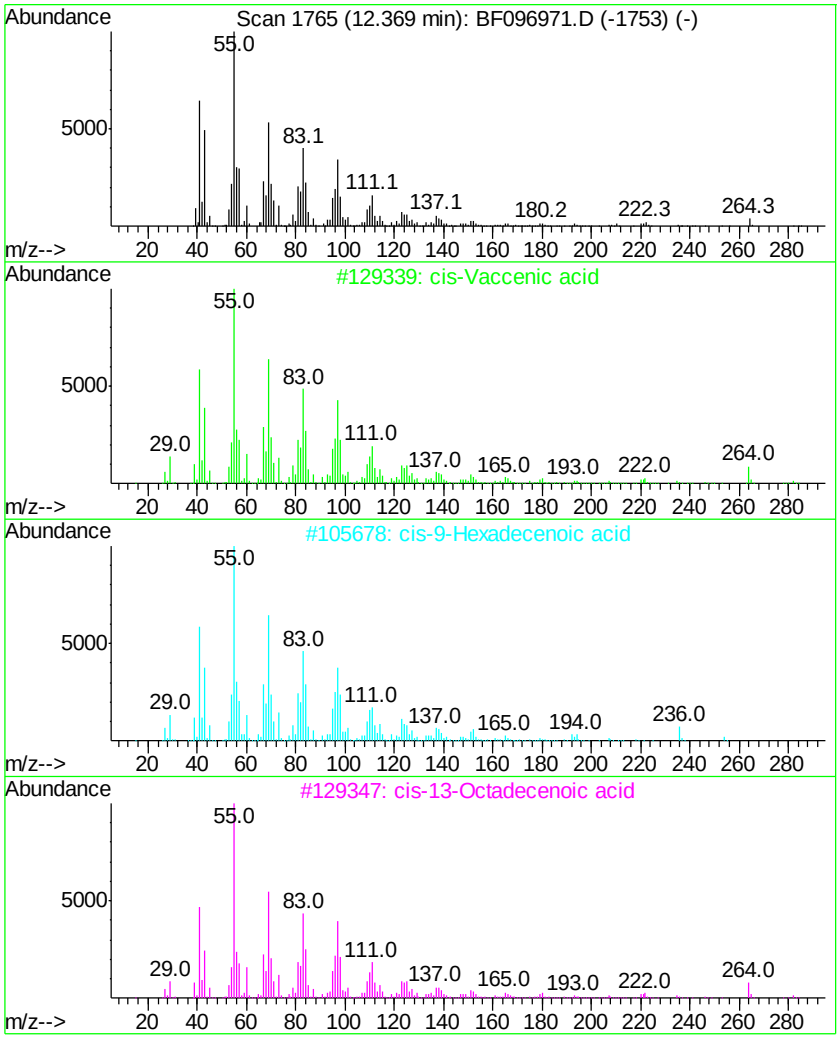
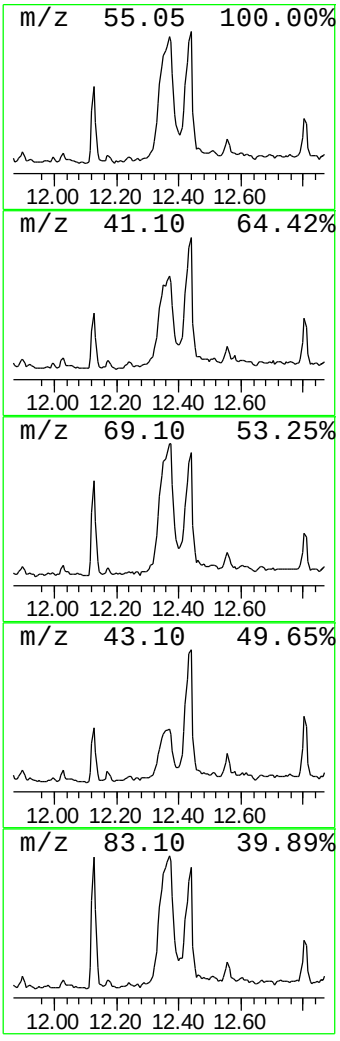
Peak Number 11 cis-Vaccenic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	102.09 ng	5569820	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
4	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	91
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	91





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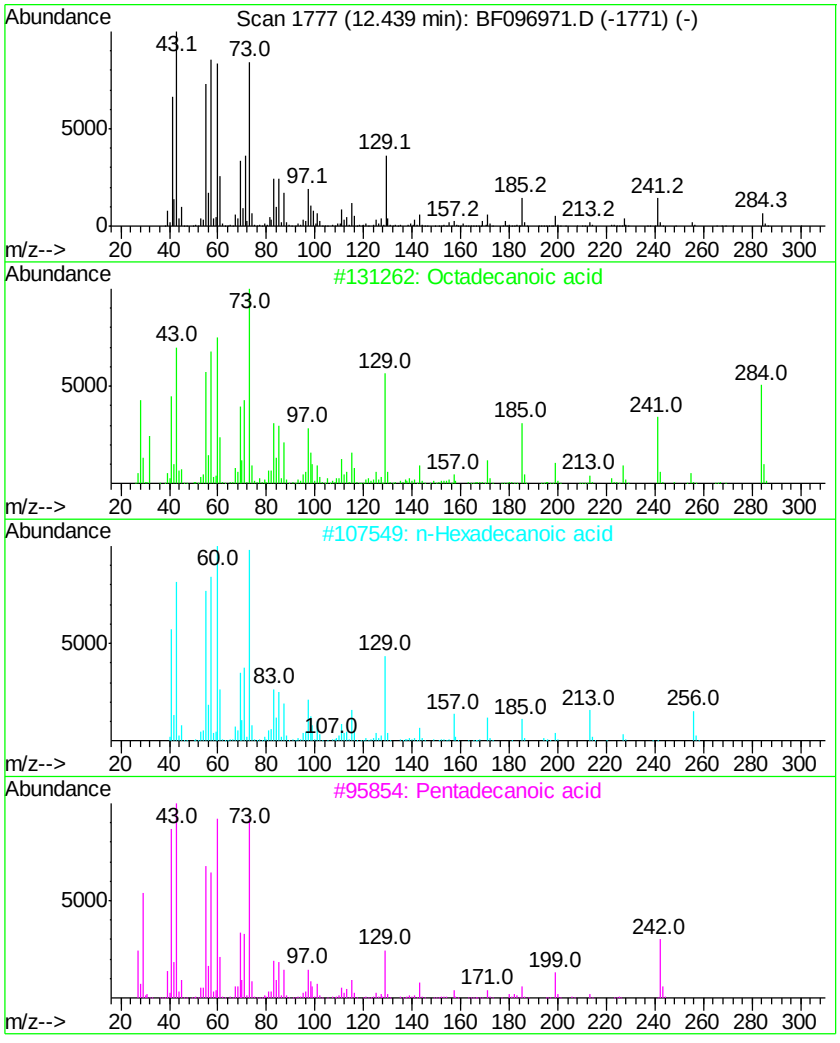
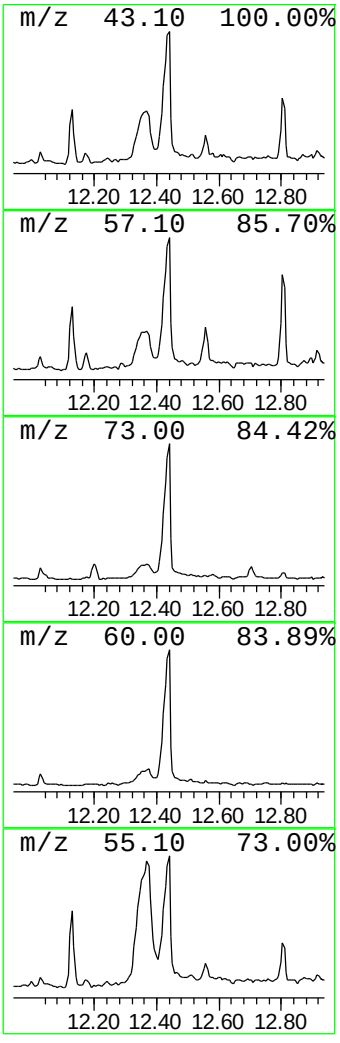
Peak Number 12 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	104.94 ng	3950360	Chrysene-d12	13.69

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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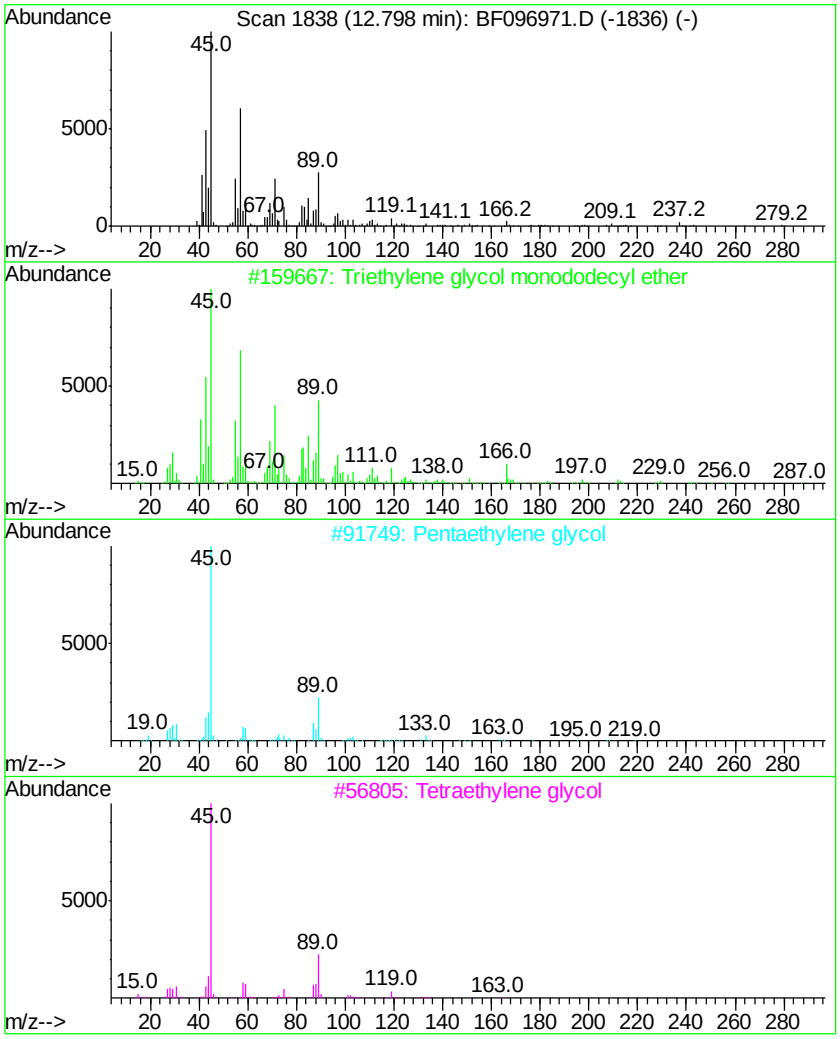
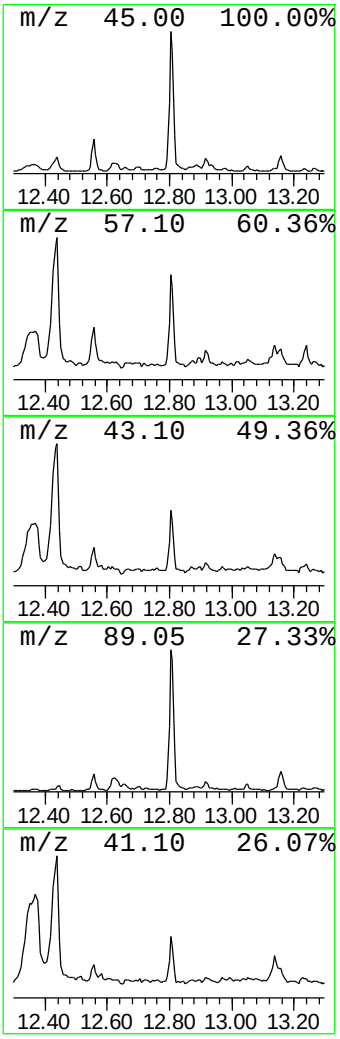
Peak Number 13 Triethylene glycol monodode... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	36.21 ng	1363070	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	91
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	58
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	53
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	53





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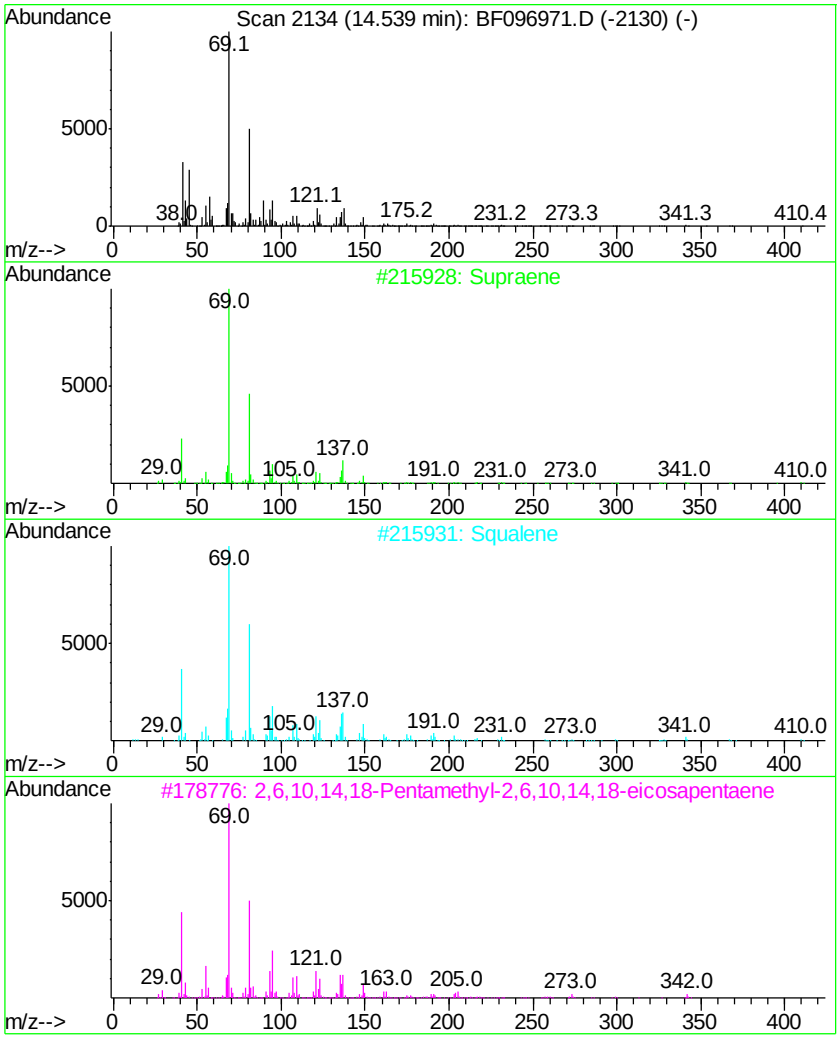
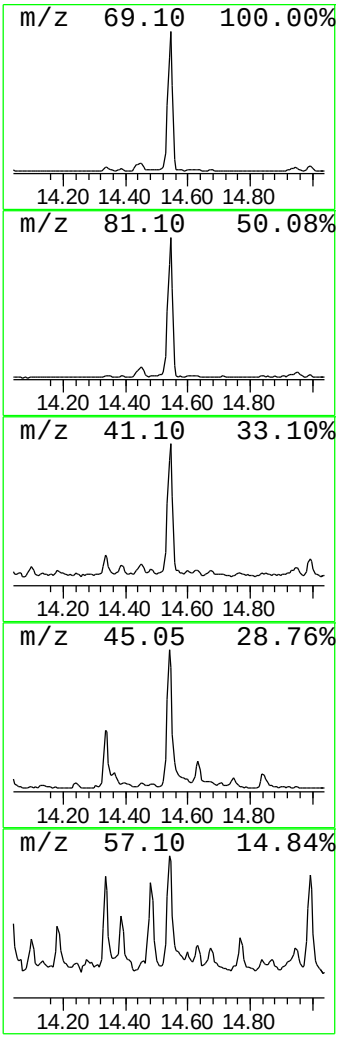
Peak Number 14 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	147.67 ng	4256610	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	76
2	Squalene	410	C30H50	000111-02-4	68
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	53
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	50
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	43





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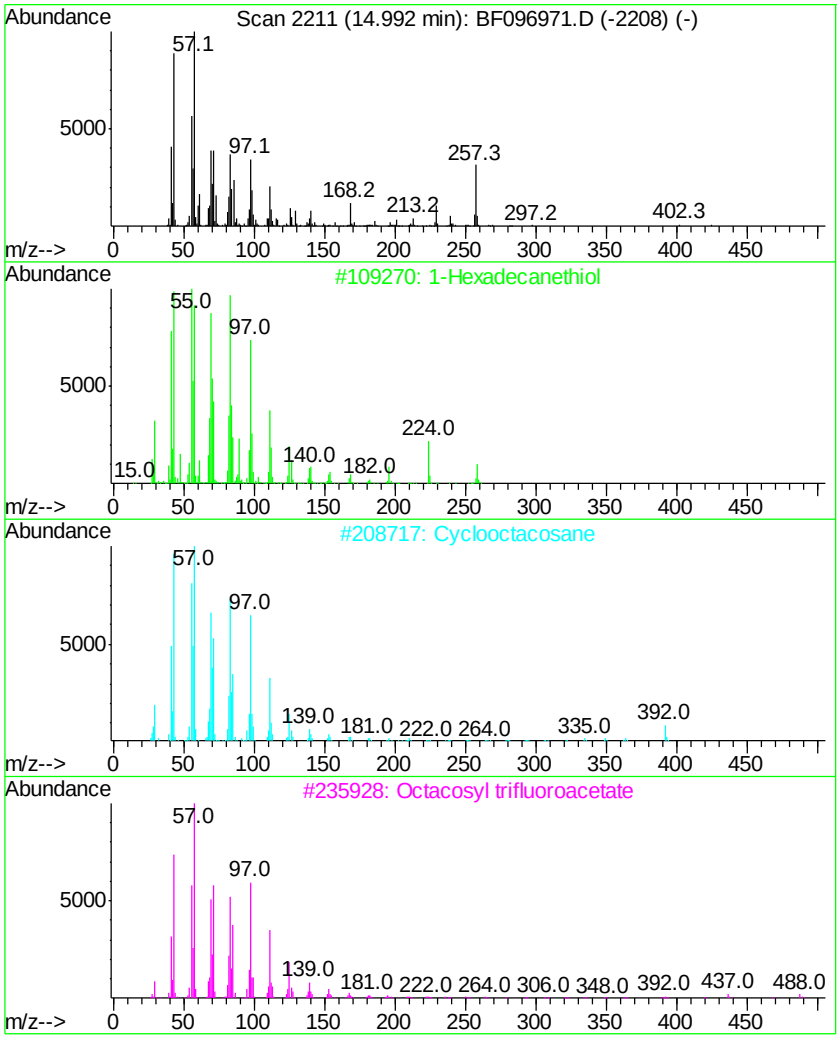
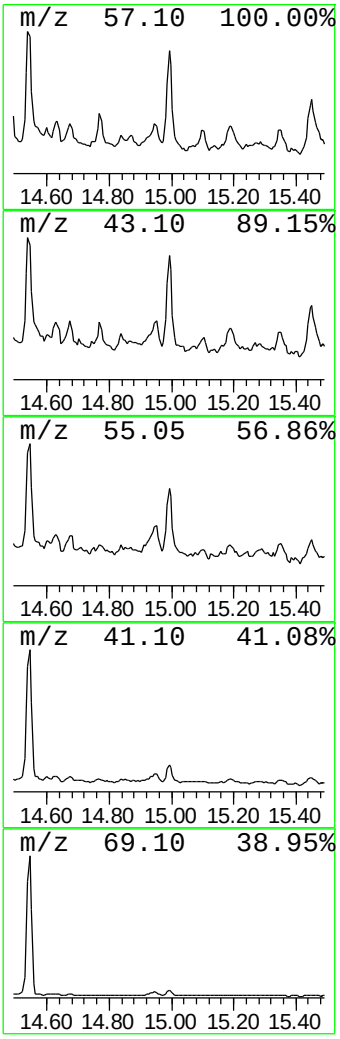
Peak Number 15 1-Hexadecanethiol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	28.97 ng	835110	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	87
2	Cyclooctacosane	392	C28H56	000297-24-5	68
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	68
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5	Heptacosyl trifluoroacetate	492	C29H55F3O2	1000351-75-8	64





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Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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

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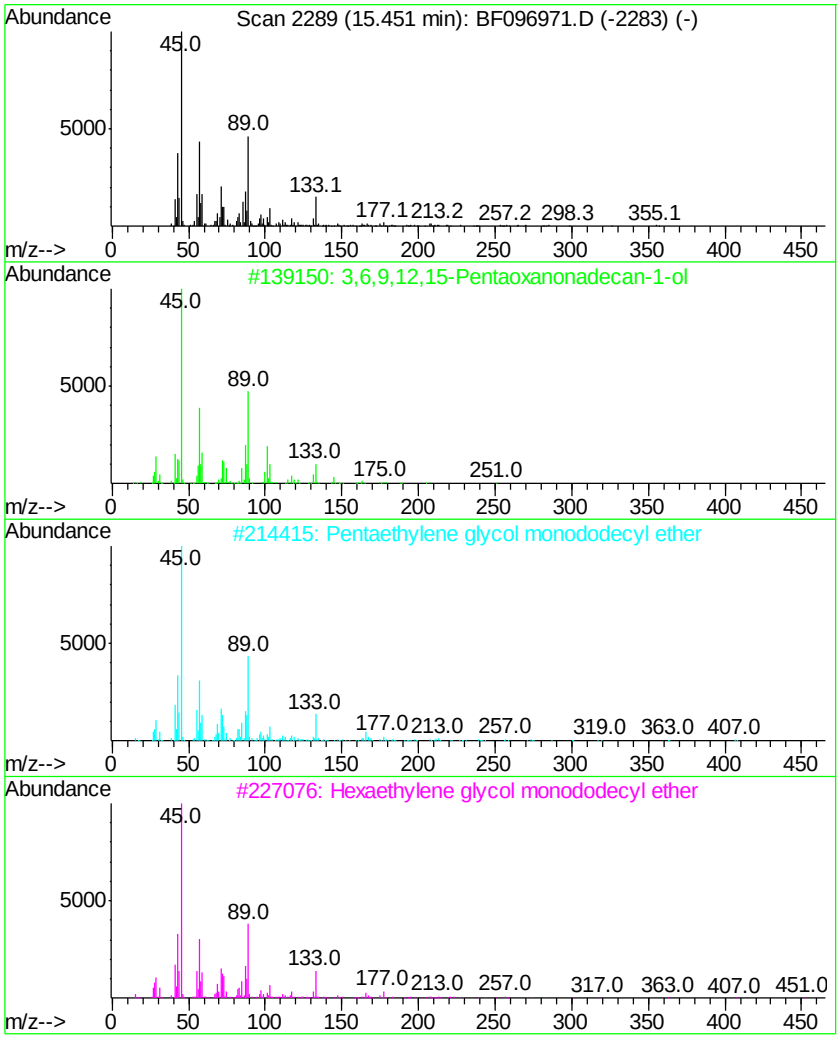
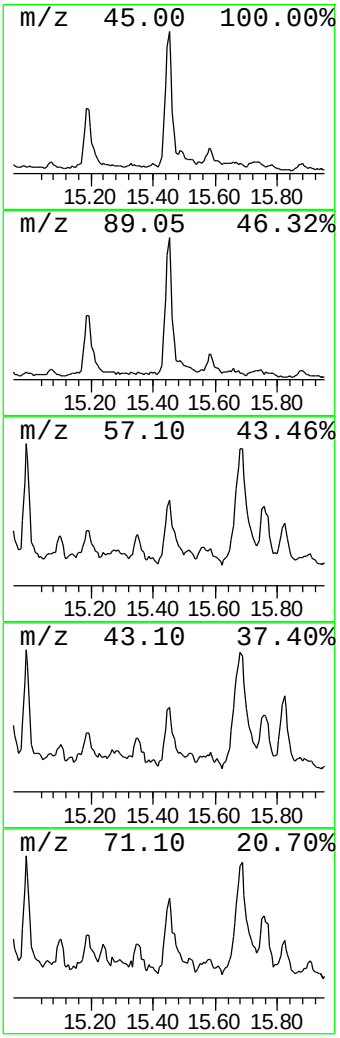
Peak Number 16 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	34.02 ng	980602	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	90
2	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	90
3	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	90
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	83
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096971.D
Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
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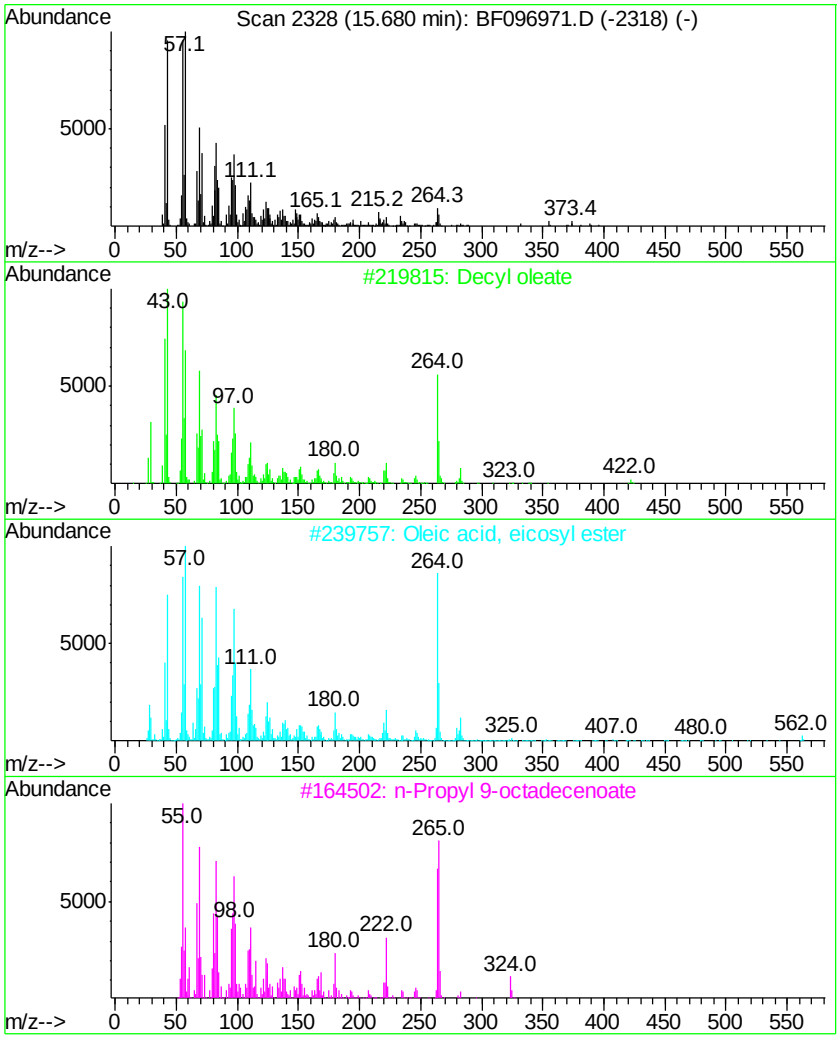
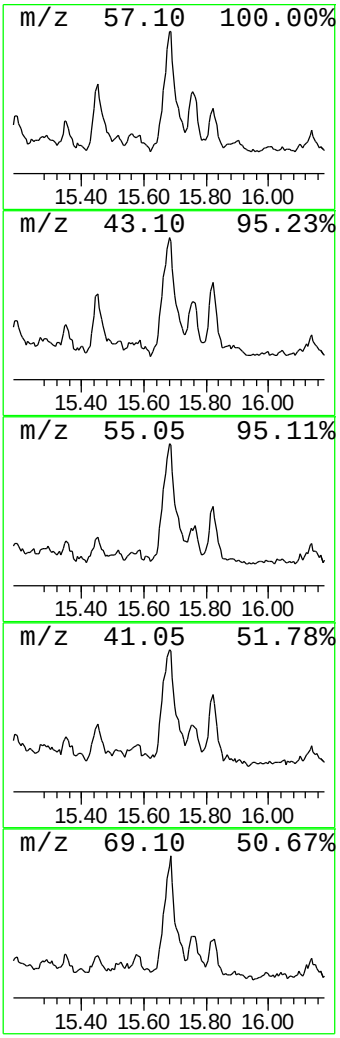
Peak Number 17 Decyl oleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	119.86 ng	3455010	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decyl oleate	422	C28H54O2	003687-46-5	83
2	Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	80
3	n-Propyl 9-octadecenoate	324	C21H40O2	1000336-71-6	74
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	72
5	Oleyl alcohol, trifluoroacetate	364	C20H35F3O2	1000352-68-4	72





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Data File : BF096971.D
Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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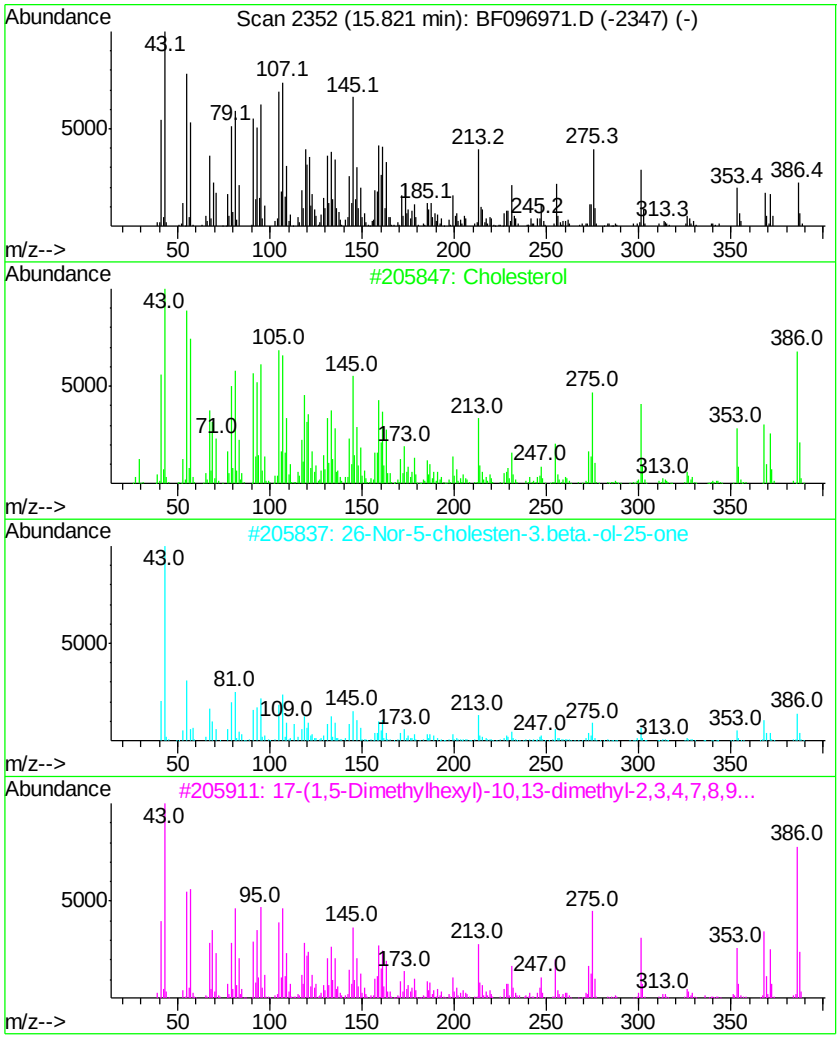
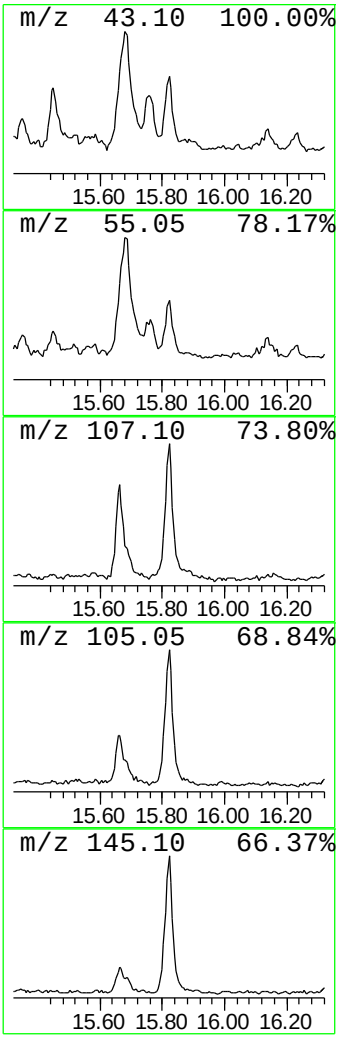
Peak Number 18 Cholesterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	56.92 ng	1640610	Perylene-d12	15.05

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	91
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	68
4	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	35
5	Pyrethrin II	372	C22H28O5	000121-29-9	25





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Acq On : 22 Jul 2017 5:34
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Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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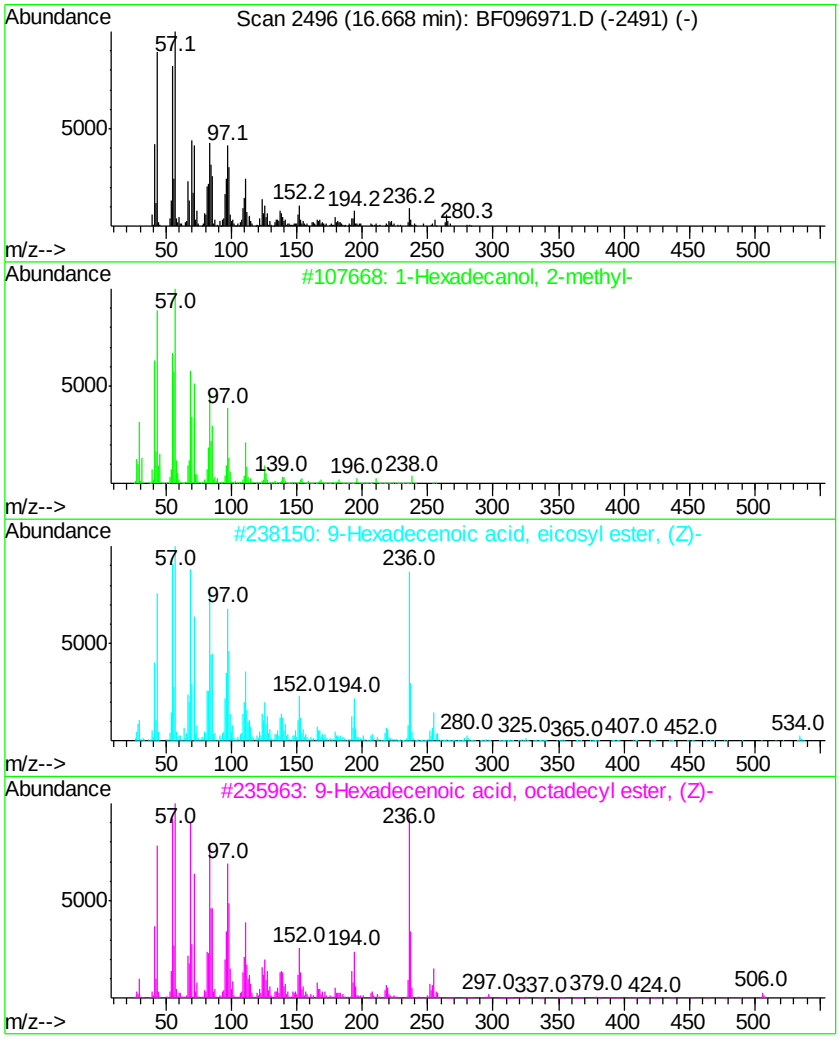
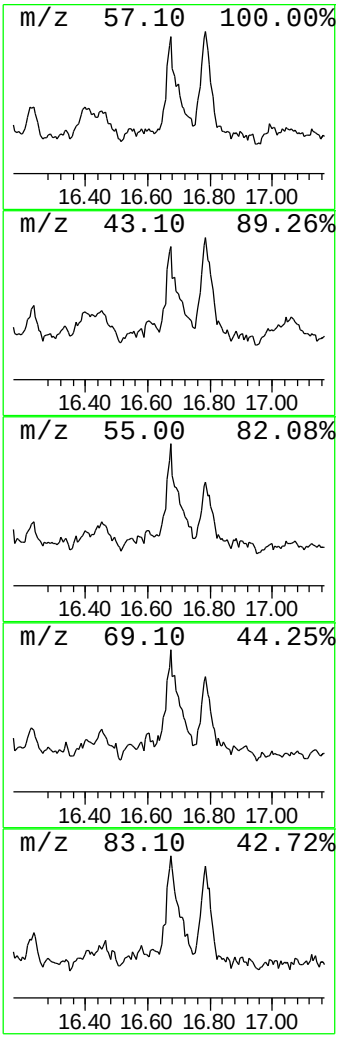
Peak Number 19 1-Hexadecanol, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	36.07 ng	1039830	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	93
2	9-Hexadecenoic acid, eicosyl est...	535	C36H70O2	022522-34-5	83
3	9-Hexadecenoic acid, octadecyl e...	507	C34H66O2	022393-84-6	83
4	17-Pentatriacontene	491	C35H70	006971-40-0	81
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	68





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096971.D
Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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

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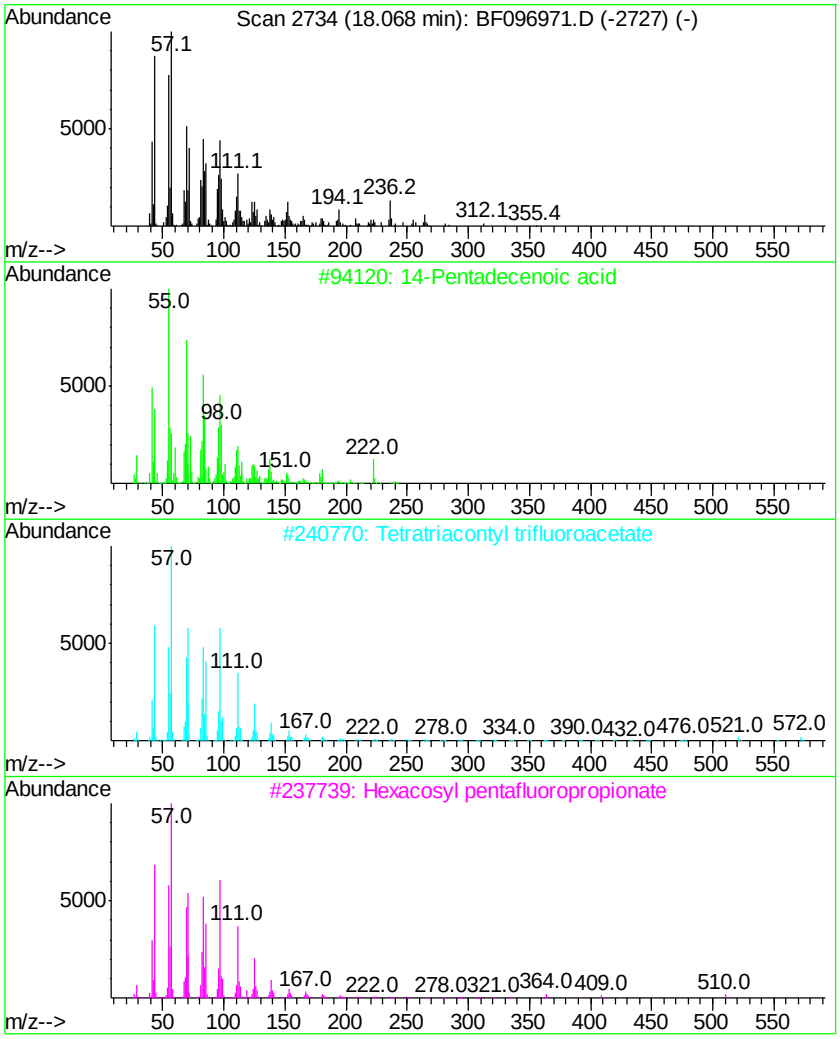
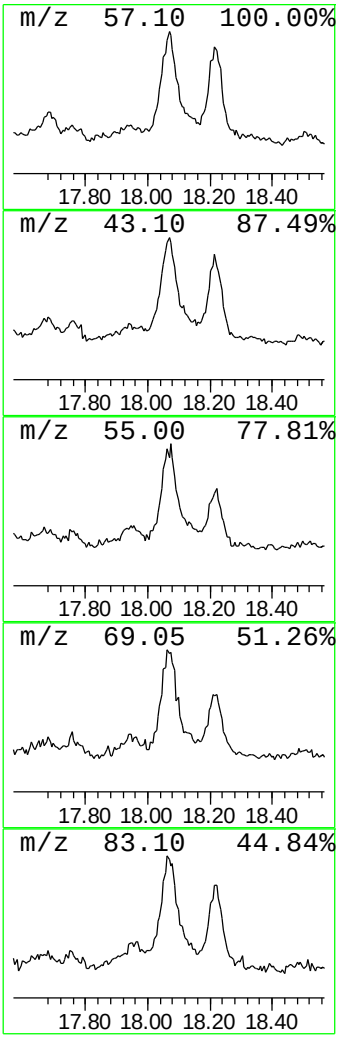
Peak Number 20 14-Pentadecenoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	27.30 ng	786964	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Pentadecenoic acid	240	C15H28O2	017351-34-7	78
2	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	76
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	76
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	76
5	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	76





Tentatively Identified Compound (LSC) summary

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Data File : BF096971.D
Acq On : 22 Jul 2017 5:34
Operator : SJ/JU
Sample : I4274-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-COMB-05

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
unknown6.33	6.33	42.9	ng	1697720	1	6.56	792001	20.0
Ethanol, 2-phenoxy-	8.01	33.7	ng	1619860	2	7.84	961553	20.0
Benzeneacetic acid	8.18	32.2	ng	1548500	2	7.84	961553	20.0
n-Decanoic acid	8.83	52.0	ng	2261040	3	9.59	870272	20.0
Cyclopropane, nonyl-	9.42	74.7	ng	3250060	3	9.59	870272	20.0
Dodecanoic acid	9.89	140.5	ng	6112430	3	9.59	870272	20.0
Dimantine	10.56	31.3	ng	1704760	4	11.06	1091180	20.0
unknown10.60	10.60	27.0	ng	1472370	4	11.06	1091180	20.0
Tetradecanoic acid	10.80	83.0	ng	4526180	4	11.06	1091180	20.0
n-Hexadecanoic acid	11.70	319.5	ng	17433700	4	11.06	1091180	20.0
cis-Vaccenic acid	12.37	102.1	ng	5569820	4	11.06	1091180	20.0
Octadecanoic acid	12.44	104.9	ng	3950360	5	13.69	752902	20.0
Triethylene glyco...	12.80	36.2	ng	1363070	5	13.69	752902	20.0
Supraene	14.54	147.7	ng	4256610	6	15.05	576501	20.0
1-Hexadecanethiol	14.99	29.0	ng	835110	6	15.05	576501	20.0
3,6,9,12,15-Penta...	15.45	34.0	ng	980602	6	15.05	576501	20.0
Decyl oleate	15.68	119.9	ng	3455010	6	15.05	576501	20.0
Cholesterol	15.82	56.9	ng	1640610	6	15.05	576501	20.0
1-Hexadecanol, 2-...	16.67	36.1	ng	1039830	6	15.05	576501	20.0
14-Pentadecenoic ...	18.07	27.3	ng	786964	6	15.05	576501	20.0