LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

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-BF110817.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	5.140	514	519	531	rVB	646694	881420	18.34%	1.792%
2	5.528	579	585	588	rBV	3589104	4129650	85.94%	8.398%
3	6.528	748	755	758	rBV	3764400	4374598	91.04%	8.896%
4	6.675	774	780	783	rBV	3790387	4193361	87.27%	8.527%
5	6.904	815	819	822	rVB	1268391	1146088	23.85%	2.331%
6	7.057	841	845	849	rVB	3426755	3205049	66.70%	6.518%
7	7.463	908	914	917	rBV	2709403	2790588	58.07%	5.675%
8	8.181	1032	1036	1043	rVB	1760242	1580966	32.90%	3.215%
9	8.733	1126	1130	1133	rBV	269333	209395	4.36%	0.426%
10	9.257	1214	1219	1222	rBV	4608199	4805300	100.00%	9.772%
11	9.645	1282	1285	1289	rVB	154584	114880	2.39%	0.234%
12	9.939	1329	1335	1338	rBV	1957656	1702058	35.42%	3.461%
13	10.651	1451	1456	1459	rBV	966794	795910	16.56%	1.619%
14	10.727	1463	1469	1472	rBV	2907580	2867637	59.68%	5.831%
15	11.422	1581	1587	1590	rBV	1765506	1758133	36.59%	3.575%
16	11.445	1590	1591	1594	rVV	543505	358875	7.47%	0.730%
17	11.498	1598	1600	1602	rVB	72538	52947	1.10%	0.108%
18	11.645	1620	1625	1628	rBV2	46866	55287	1.15%	0.112%
19	11.945	1669	1676	1683	rBV2	528818	699696	14.56%	1.423%
20	12.033	1687	1691	1693	rVV2	115377	126903	2.64%	0.258%
21	12.057	1693	1695	1698	rVB	75435	58335	1.21%	0.119%
22	12.216	1719	1722	1724	rBV	71968	69023	1.44%	0.140%
23	12.239	1724	1726	1729	rVB	87673	64913	1.35%	0.132%
24	12.469	1763	1765	1768	rVB	77639	72879	1.52%	0.148%
25	12.557	1777	1780	1785	rVB	66819	75341	1.57%	0.153%
26	12.633	1790	1793	1798	rVV	976875	858382	17.86%	1.746%
27	12.727	1806	1809	1812	rBV	278305	248866	5.18%	0.506%
28	12.863	1826	1832	1837	rBV2	823077	892036	18.56%	1.814%
29	12.910	1837	1840	1846	rVB3	61627	90149	1.88%	0.183%
30	12.980	1849	1852	1853	rBV	56227	49305	1.03%	0.100%
31	13.010	1853	1857	1860	rVV	3935143	3981987	82.87%	8.098%
32	13.080	1864	1869	1873	rBV3	74066	131404	2.73%	0.267%
33	13.168	1880	1884	1885	rBV3	57415	58448	1.22%	0.119%
34	13.192	1885	1888	1892	rVB	104089	105439	2.19%	0.214%

LSC Area Percent Report

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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.292	1901	1905	1908	rBV2	103885	110212	2.29%	0.224%
36	13.386	1919	1921	1924	rVB	58397	49245	1.02%	0.100%
37	13.415	1924	1926	1930	rBV2	61930	63331	1.32%	0.129%
38	13.580	1948	1954	1955	rBV5	35230	71999	1.50%	0.146%
39	13.692	1971	1973	1978	rVB	96825	100807	2.10%	0.205%
40	13.810	1988	1993	1996	rBV2	75079	121554	2.53%	0.247%
41	13.839	1996	1998	2000	rVV	91597	79468	1.65%	0.162%
42	13.863	2000	2002	2005	rVV2	58948	84760	1.76%	0.172%
43	13.892	2005	2007	2015	rVB2	291890	340251	7.08%	0.692%
44	14.063	2030	2036	2038	rBV2	1384664	1557156	32.40%	3.167%
45	14.086	2038	2040	2045	rVB	446952	381377	7.94%	0.776%
46	14.286	2070	2074	2076	rBV2	37408	59748	1.24%	0.122%
47	14.445	2098	2101	2104	rVB	96765	86241	1.79%	0.175%
48	14.480	2104	2107	2110	rVB2	78356	76277	1.59%	0.155%
49	14.527	2111	2115	2120	rBV4	95020	128057	2.66%	0.260%
50	14.915	2178	2181	2184	rBV3	33371	48306	1.01%	0.098%
51	15.104	2209	2213	2217	rBV	337562	565400	11.77%	1.150%
52	15.215	2228	2232	2236	rVB	77276	96526	2.01%	0.196%
53	15.321	2244	2250	2252	rBV5	36168	70912	1.48%	0.144%
54	15.415	2262	2266	2272	rVB	226603	271286	5.65%	0.552%
55	15.474	2272	2276	2282	rVB	290239	366755	7.63%	0.746%
56	15.545	2282	2288	2292	rBV	881764	1142337	23.77%	2.323%
57	17.027	2534	2540	2548	rVB2	153269	329416	6.86%	0.670%
58	17.215	2568	2572	2577	rBV	35206	56534	1.18%	0.115%
59	17.480	2611	2617	2627	rVB	117130	246722	5.13%	0.502%
60	17.639	2639	2644	2651	rVB10	31412	65261	1.36%	0.133%

Sum of corrected areas: 49175186

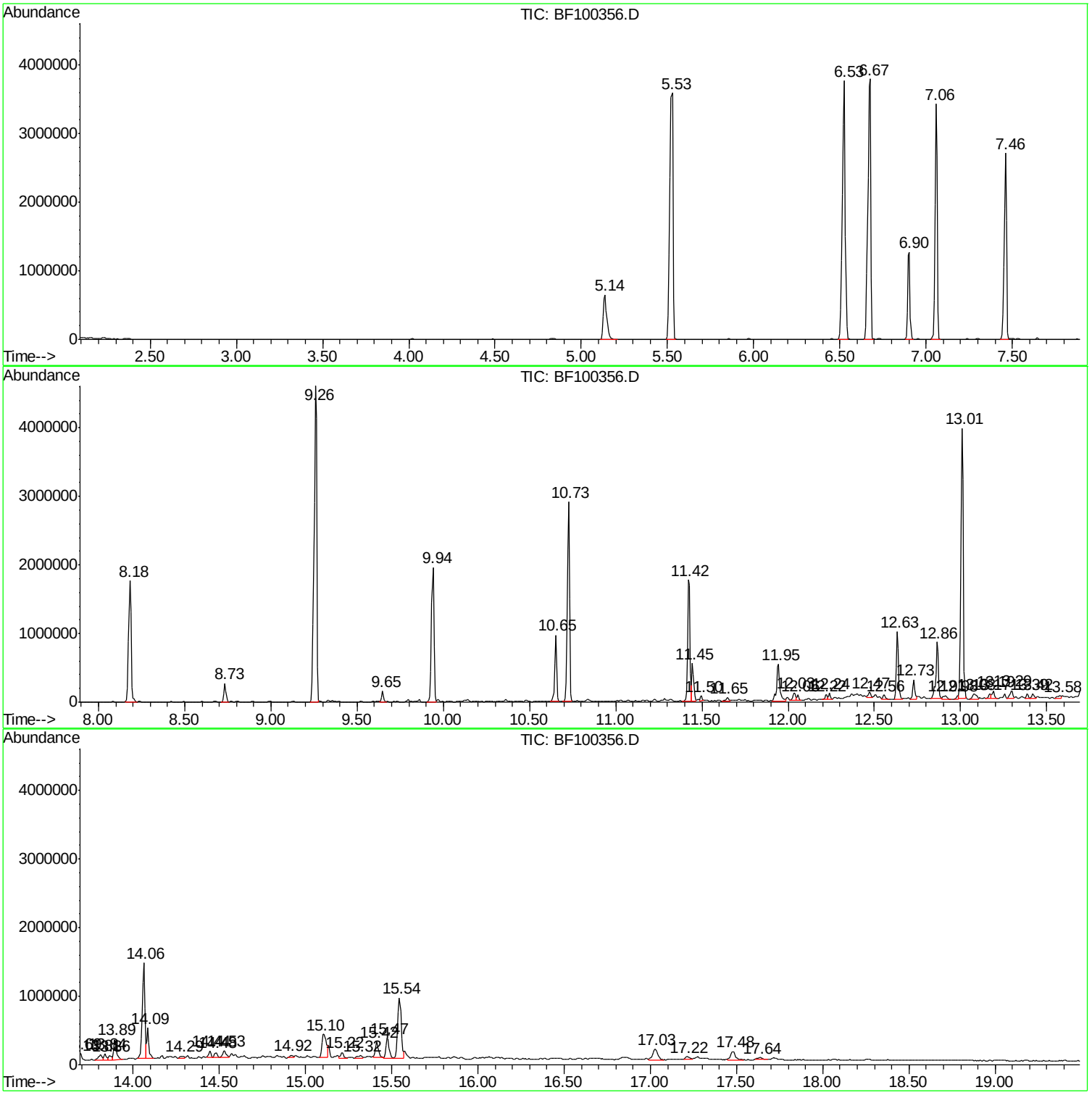
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
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Misc :
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Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

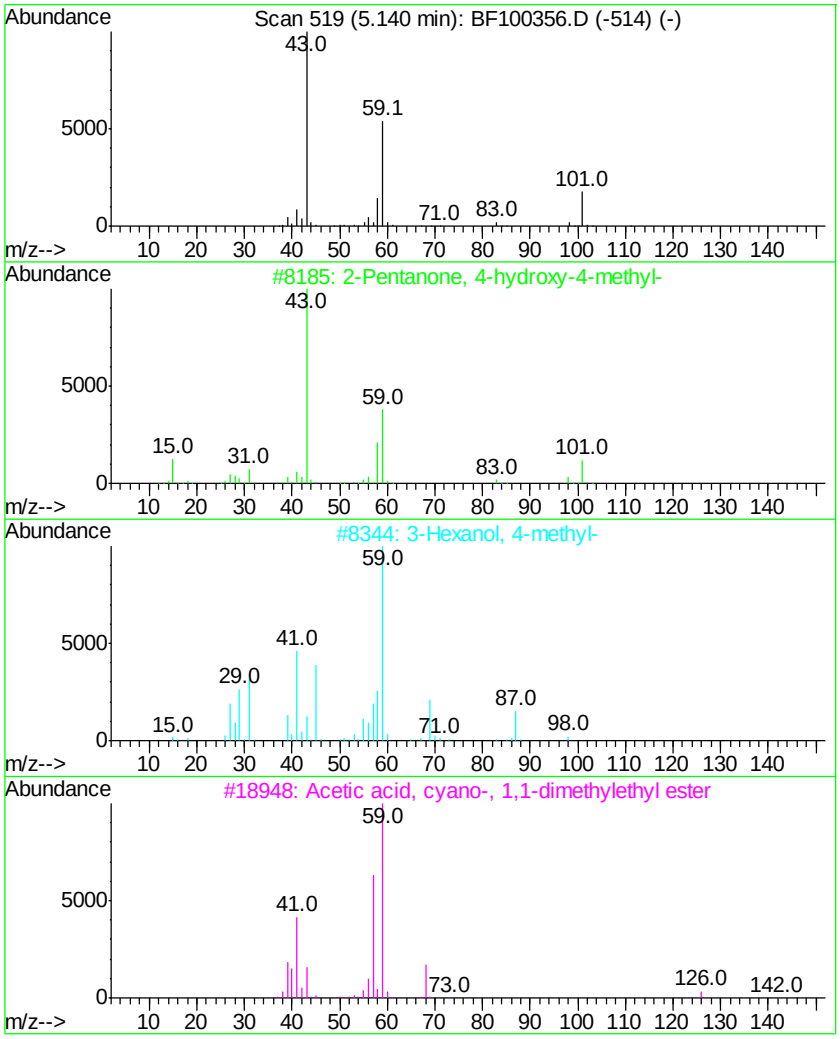
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

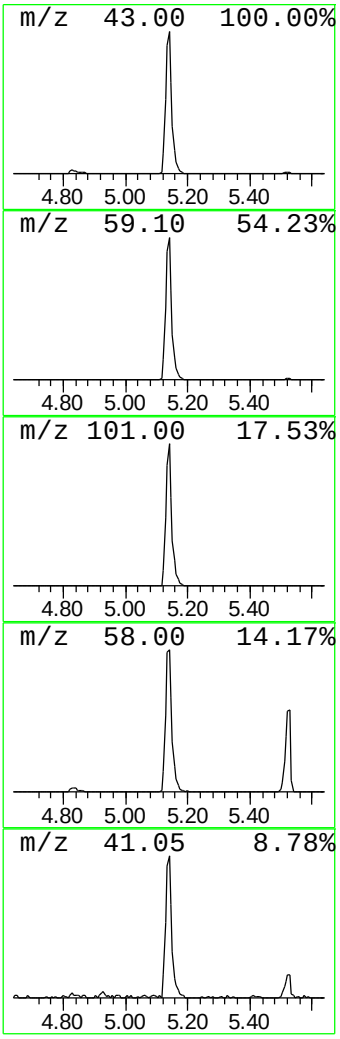
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	15.38 ng	881420	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

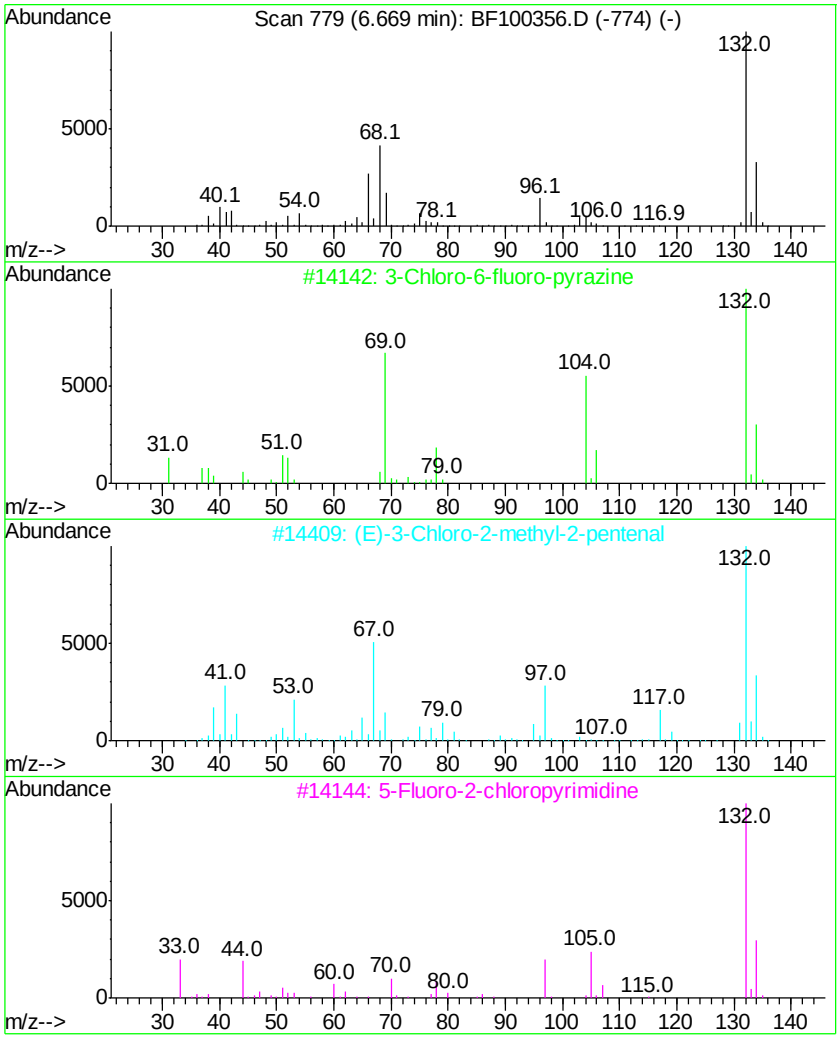
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

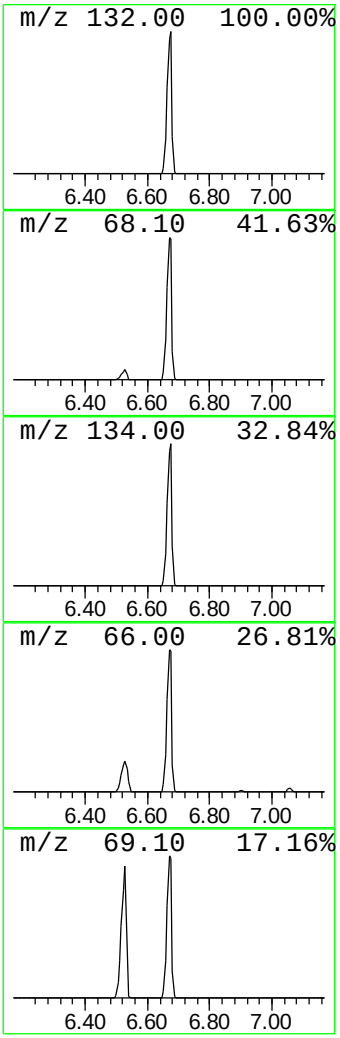
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	73.18 ng	4193360	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Data File : BF100356.D
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Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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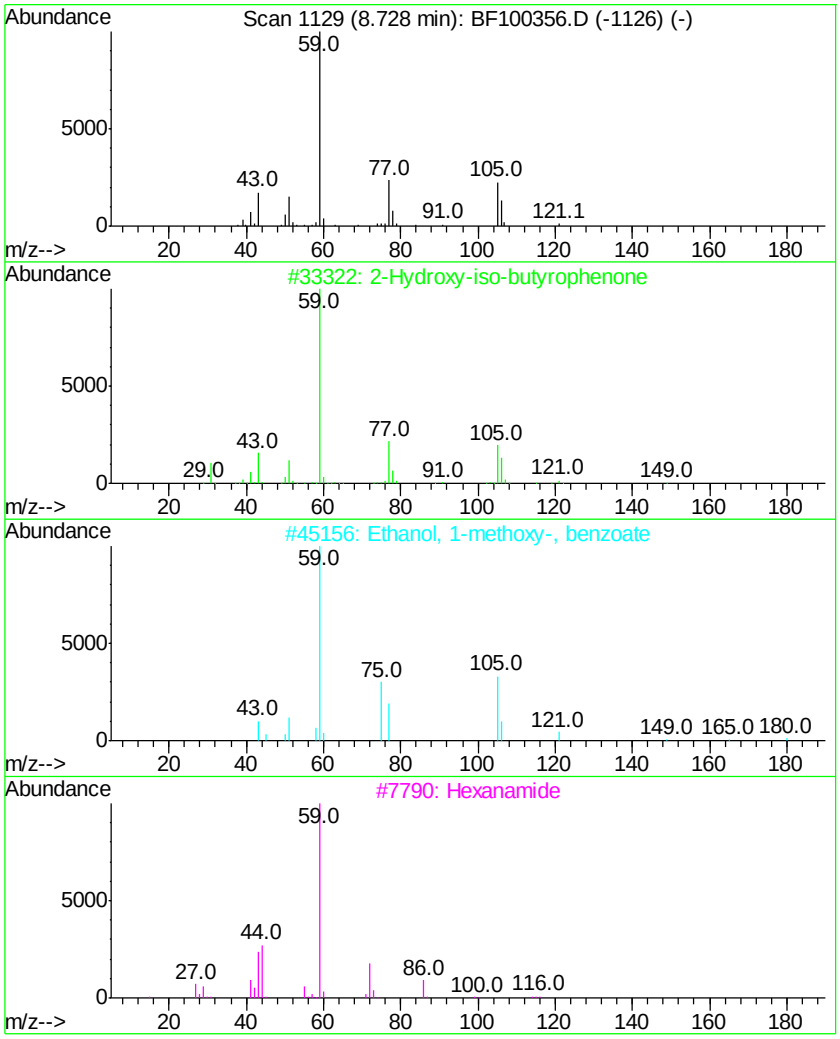
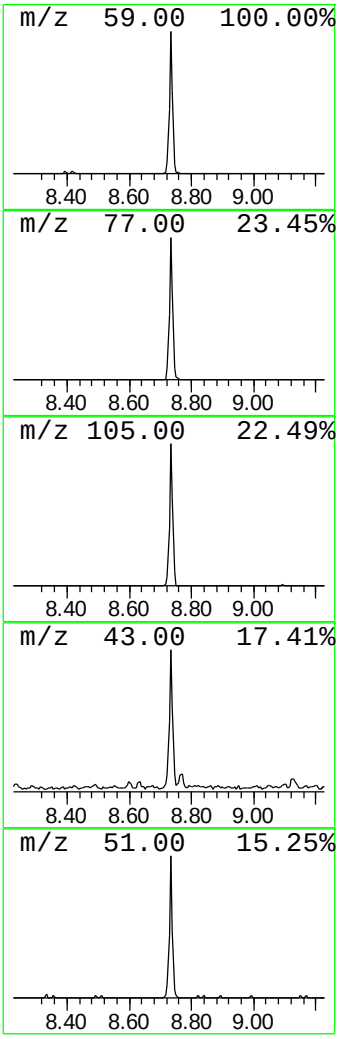
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.65 ng	209395	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Hexanamide	115	C6H13NO	000628-02-4	9
4	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
5	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
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Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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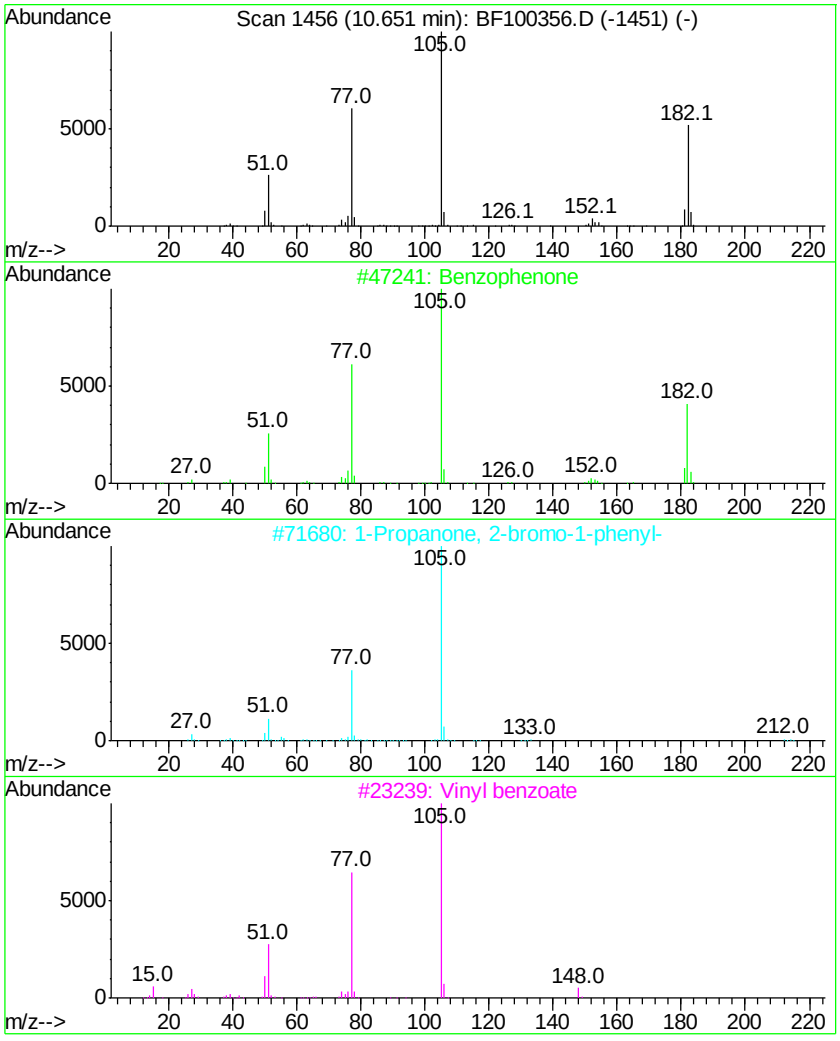
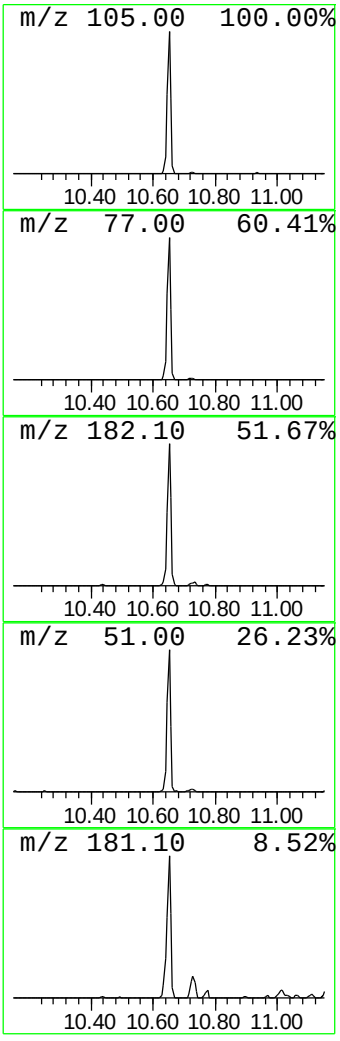
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	9.35 ng	795910	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Library Search Compound Report

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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
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Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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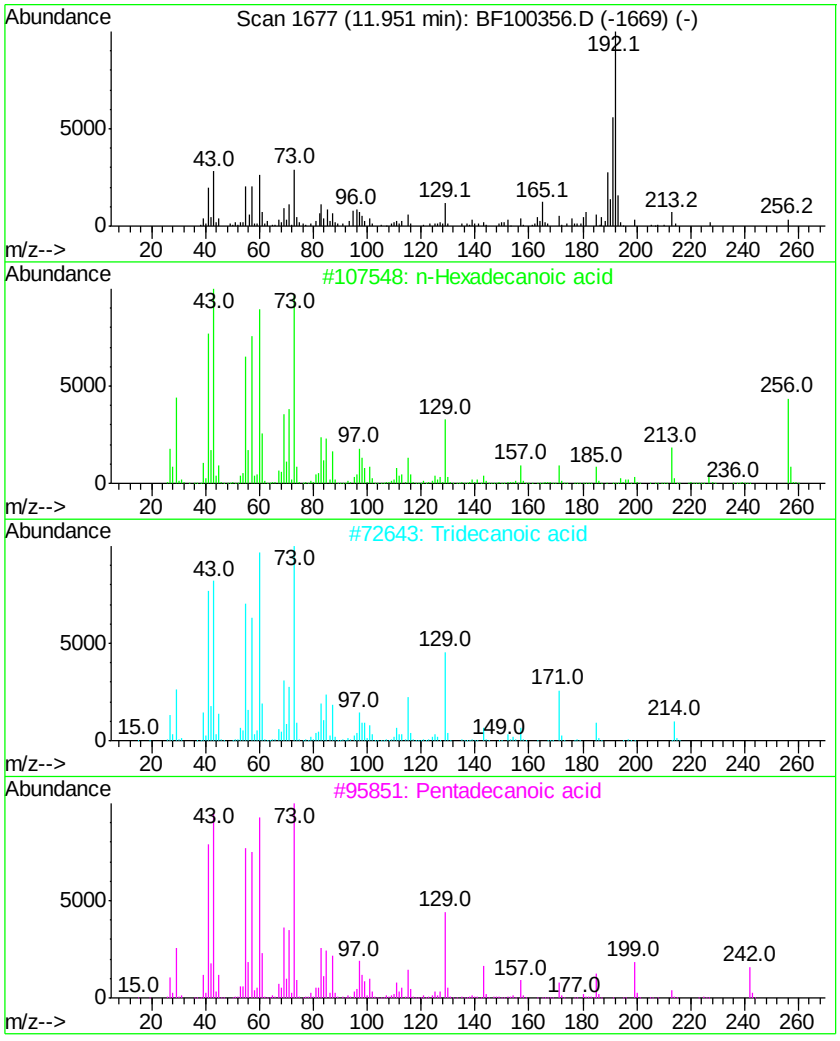
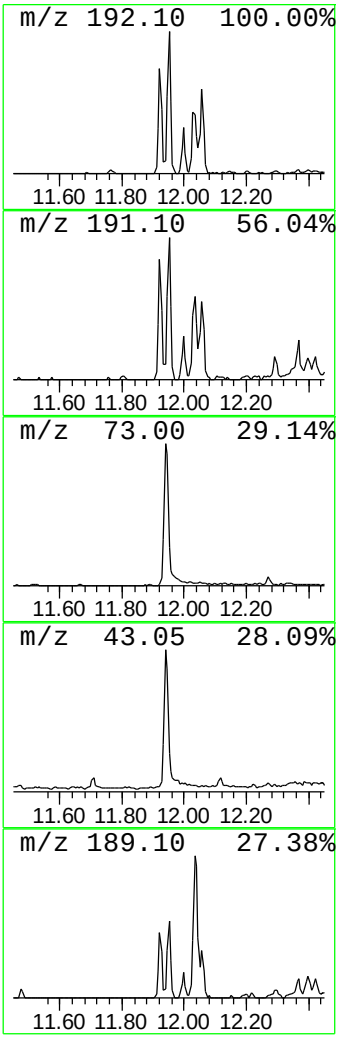
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	7.96 ng	699696	Phenanthrene-d10	11.42

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BF100356.D
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Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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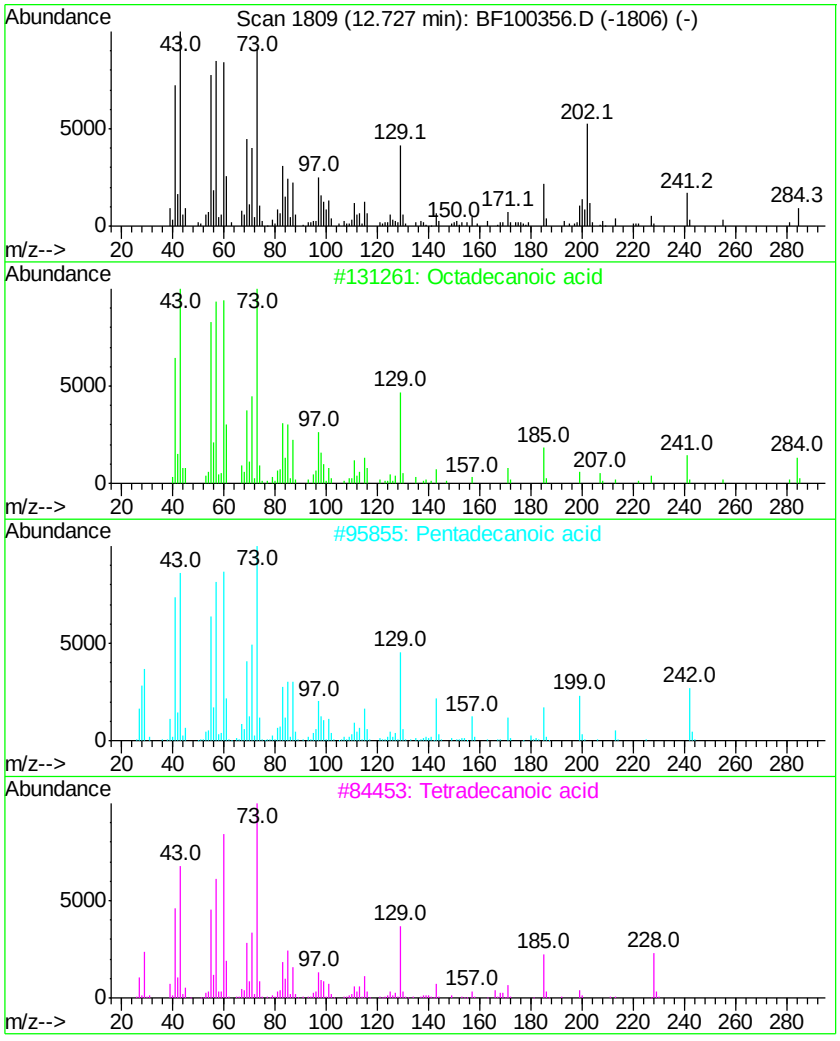
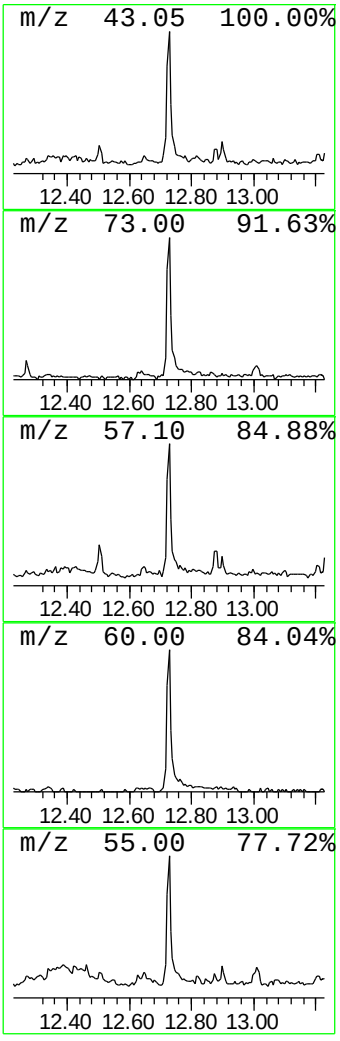
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.83 ng	248866	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	55





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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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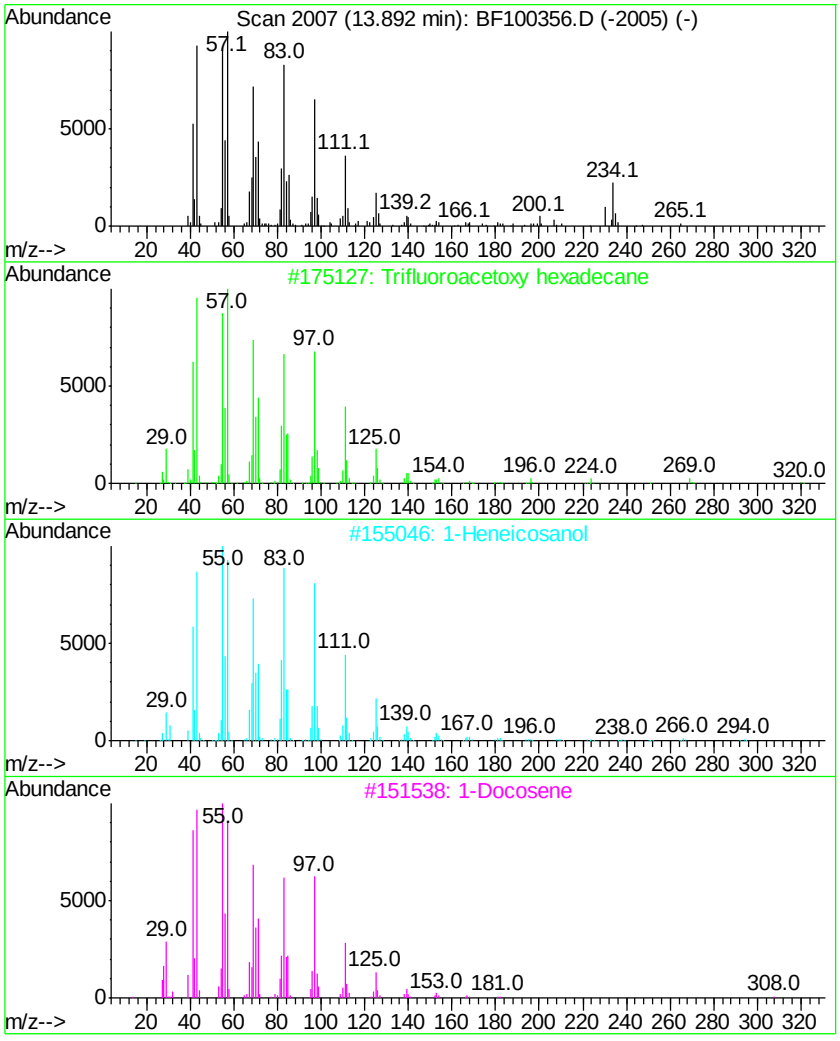
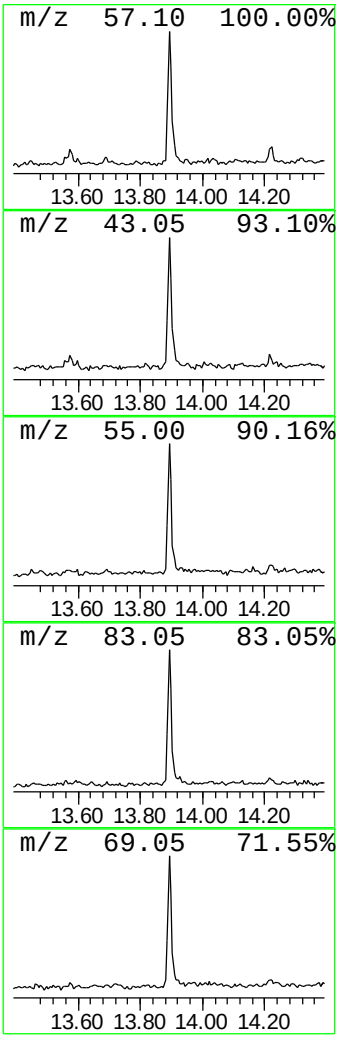
Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	4.37 ng	340251	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	89





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Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
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Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

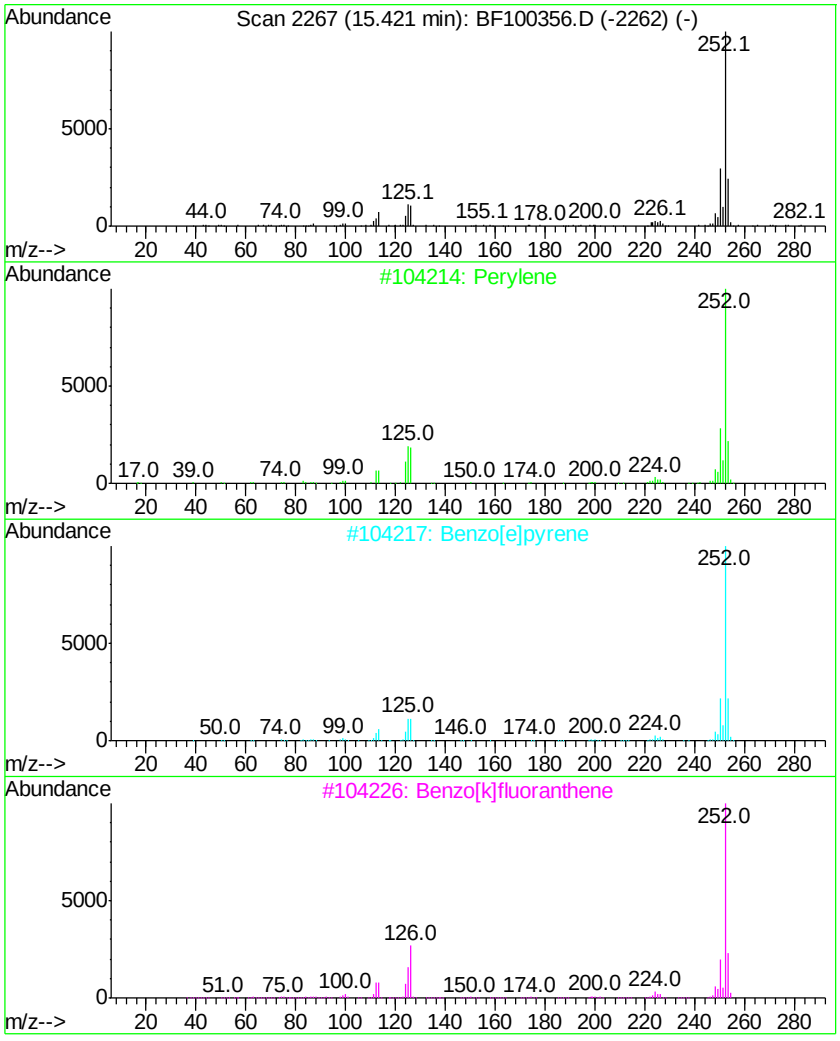
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

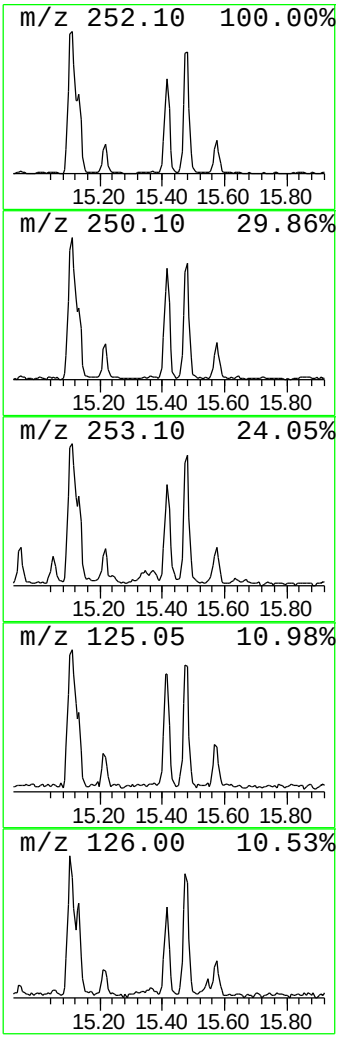
****

Peak Number 9 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	4.75 ng	271286	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF110917\
Data File : BF100356.D
Acq On : 9 Nov 2017 22:23
Operator : SJ/JU
Sample : I6379-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1-(2-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
2-Pentanone, 4-hy...	5.14	15.4	ng	881420	1	6.90	1146090	20.0
unknown6.67	6.67	73.2	ng	4193360	1	6.90	1146090	20.0
2-Hydroxy-iso-but...	8.73	2.6	ng	209395	2	8.18	1580970	20.0
Benzophenone	10.65	9.3	ng	795910	3	9.94	1702060	20.0
n-Hexadecanoic acid	11.95	8.0	ng	699696	4	11.42	1758130	20.0
Octadecanoic acid	12.73	2.8	ng	248866	4	11.42	1758130	20.0
Trifluoroacetoxy ...	13.89	4.4	ng	340251	5	14.06	1557160	20.0
Perylene	15.42	4.8	ng	271286	6	15.54	1142340	20.0