LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117564.D
Acq On : 28 Oct 2019 16:31
Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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	5.351	552	555	574	rBV	522288	692540	81.63%	7.098%
2	6.381	726	730	747	rBV	679866	796481	93.88%	8.163%
3	6.504	747	751	771	rVB	815135	840931	99.12%	8.619%
4	6.728	785	789	799	rBV	213323	212668	25.07%	2.180%
5	6.881	811	815	830	rBV	685241	609201	71.81%	6.244%
6	7.292	882	885	903	rBV	422078	480086	56.59%	4.920%
7	8.010	1003	1007	1024	rBV	239293	280462	33.06%	2.874%
8	9.080	1185	1189	1202	rBV	959827	848408	100.00%	8.695%
9	9.480	1253	1257	1271	rVB	98012	100729	11.87%	1.032%
10	9.757	1301	1304	1308	rBV	358123	310974	36.65%	3.187%
11	9.786	1308	1309	1318	rVB	16552	18458	2.18%	0.189%
12	10.316	1396	1399	1406	rBB	12458	13107	1.54%	0.134%
13	10.551	1436	1439	1452	rBV	440006	439509	51.80%	4.504%
14	11.245	1554	1557	1559	rBV	301161	263871	31.10%	2.704%
15	11.269	1559	1561	1567	rVV	209953	197223	23.25%	2.021%
16	11.327	1567	1571	1576	rVB	32356	37245	4.39%	0.382%
17	11.492	1594	1599	1604	rBV3	14954	19415	2.29%	0.199%
18	11.751	1640	1643	1645	rBV	18773	17342	2.04%	0.178%
19	11.774	1645	1647	1654	rVB3	58545	67719	7.98%	0.694%
20	11.863	1659	1662	1665	rBV	32413	34000	4.01%	0.348%
21	12.045	1691	1693	1698	rVB	12512	9530	1.12%	0.098%
22	12.092	1698	1701	1705	rBV	9279	9598	1.13%	0.098%
23	12.298	1732	1736	1739	rBV	13100	12691	1.50%	0.130%
24	12.398	1748	1753	1757	rVB3	9681	10730	1.26%	0.110%
25	12.463	1761	1764	1770	rVV	350113	305383	35.99%	3.130%
26	12.557	1777	1780	1785	rVB2	8375	9166	1.08%	0.094%
27	12.692	1797	1803	1810	rBV	257354	305337	35.99%	3.129%
28	12.745	1810	1812	1817	rVB2	11169	10938	1.29%	0.112%
29	12.827	1822	1826	1829	rVV	643296	562880	66.35%	5.769%
30	12.863	1829	1832	1836	rVV	9745	13643	1.61%	0.140%
31	12.910	1836	1840	1844	rVB3	14292	21845	2.57%	0.224%
32	12.998	1852	1855	1856	rBV2	11265	11228	1.32%	0.115%
33	13.021	1856	1859	1862	rVB2	25478	26612	3.14%	0.273%
34	13.086	1868	1870	1873	rBV	21741	18212	2.15%	0.187%

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Misc :
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Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.127	1873	1877	1881	rBV3	17265	23447	2.76%	0.240%
36	13.215	1889	1892	1895	rBV2	11523	12424	1.46%	0.127%
37	13.251	1895	1898	1902	rVV3	15392	17912	2.11%	0.184%
38	13.292	1903	1905	1912	rVB2	11686	14667	1.73%	0.150%
39	13.545	1944	1948	1954	rVB	15543	18561	2.19%	0.190%
40	13.645	1961	1965	1967	rBV3	21735	27286	3.22%	0.280%
41	13.662	1967	1968	1971	rVV	20786	14268	1.68%	0.146%
42	13.692	1971	1973	1975	rVV	18164	19184	2.26%	0.197%
43	13.727	1975	1979	1990	rVB5	72156	147506	17.39%	1.512%
44	13.857	1999	2001	2002	rBV	19931	15806	1.86%	0.162%
45	13.892	2002	2007	2010	rVV2	262782	400916	47.26%	4.109%
46	13.915	2010	2011	2018	rVB	125740	115307	13.59%	1.182%
47	13.998	2023	2025	2028	rVB	25076	21800	2.57%	0.223%
48	14.062	2034	2036	2040	rVB3	11161	12067	1.42%	0.124%
49	14.115	2040	2045	2046	rBV2	7329	9946	1.17%	0.102%
50	14.286	2069	2074	2078	rBV2	25160	34864	4.11%	0.357%
51	14.351	2083	2085	2087	rVV2	20879	21352	2.52%	0.219%
52	14.392	2087	2092	2094	rVV5	20977	41544	4.90%	0.426%
53	14.415	2094	2096	2098	rVV3	15653	17890	2.11%	0.183%
54	14.480	2102	2107	2111	rVB6	7985	15659	1.85%	0.160%
55	14.627	2127	2132	2134	rBV6	12922	18971	2.24%	0.194%
56	14.657	2134	2137	2139	rVB2	12918	12577	1.48%	0.129%
57	14.721	2145	2148	2152	rVB	109408	106734	12.58%	1.094%
58	14.786	2154	2159	2163	rBV7	22105	32955	3.88%	0.338%
59	14.933	2179	2184	2187	rBV	147624	217840	25.68%	2.233%
60	15.039	2195	2202	2209	rVB3	30978	60052	7.08%	0.615%
61	15.121	2213	2216	2220	rBV5	8227	12129	1.43%	0.124%
62	15.221	2229	2233	2239	rVB	78754	88373	10.42%	0.906%
63	15.280	2239	2243	2248	rBV	112704	133110	15.69%	1.364%
64	15.339	2248	2253	2256	rBV	172213	214983	25.34%	2.203%
65	15.509	2279	2282	2286	rBV5	11478	18776	2.21%	0.192%
66	15.733	2315	2320	2324	rBV2	17393	29180	3.44%	0.299%
67	15.815	2329	2334	2338	rVV6	15717	31071	3.66%	0.318%
68	16.233	2402	2405	2409	rVB2	9727	13748	1.62%	0.141%
69	16.756	2488	2494	2502	rVB2	38888	79640	9.39%	0.816%
70	16.974	2527	2531	2537	rBV7	8697	15253	1.80%	0.156%
71	17.186	2561	2567	2574	rBV3	27222	61201	7.21%	0.627%

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Instrument :
BNA_F
ClientSampleId :
187-30-(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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Sum of corrected areas: 9757161

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
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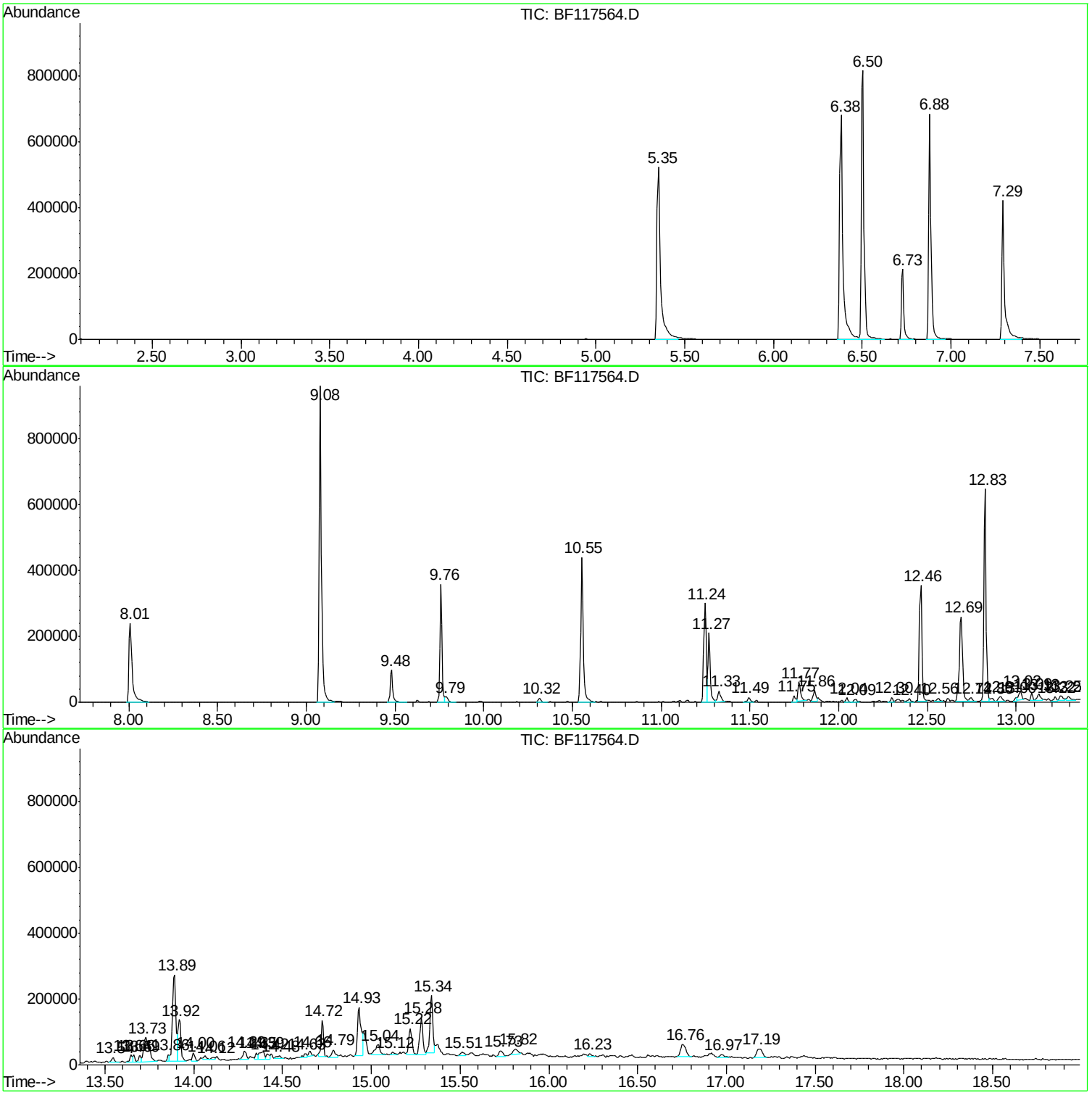
Acq On : 28 Oct 2019 16:31
Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117564.D
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Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

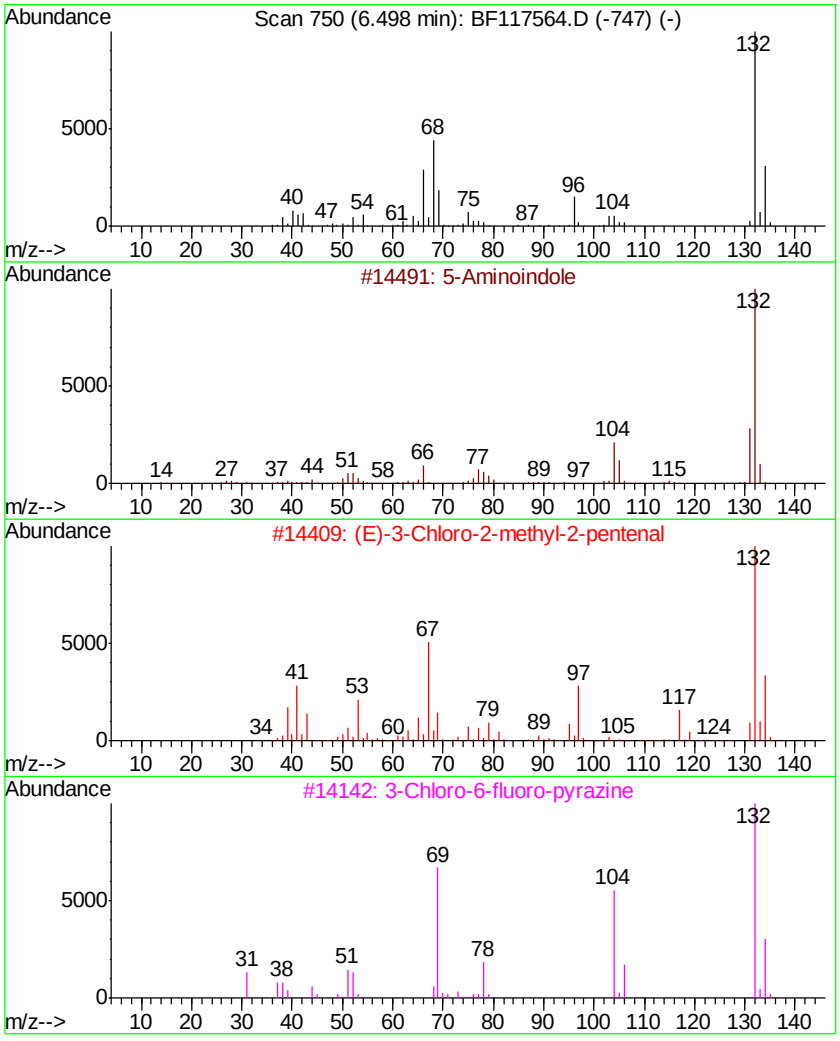
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

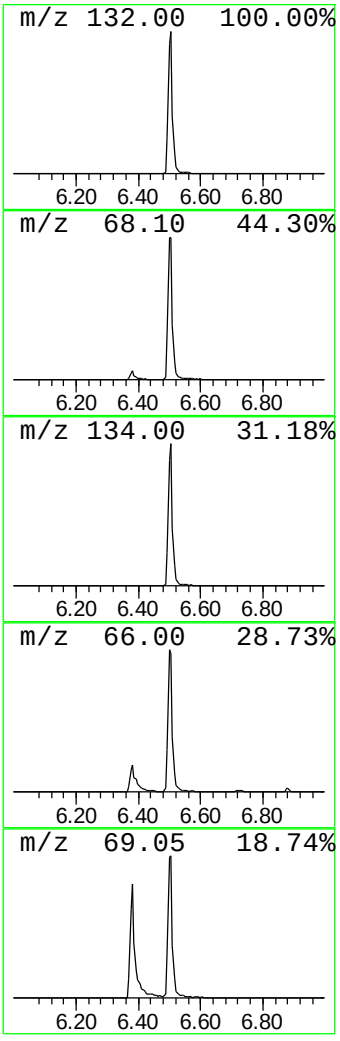
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	79.08 ng	840931	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

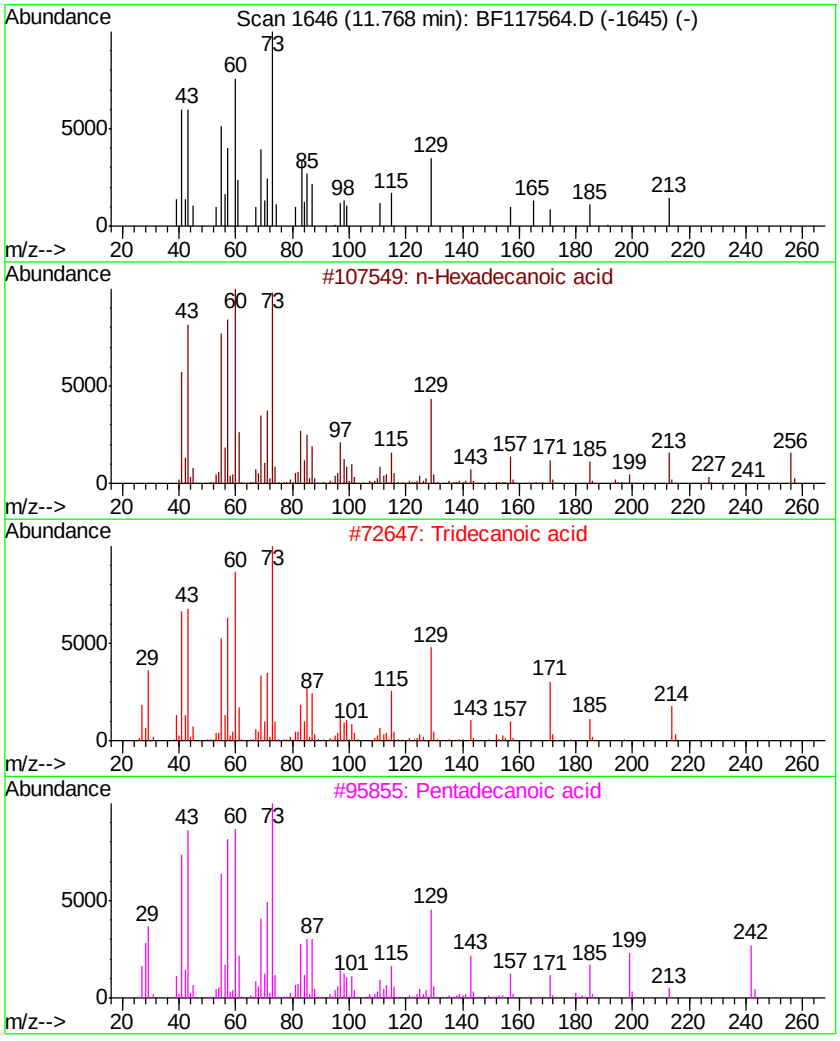
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

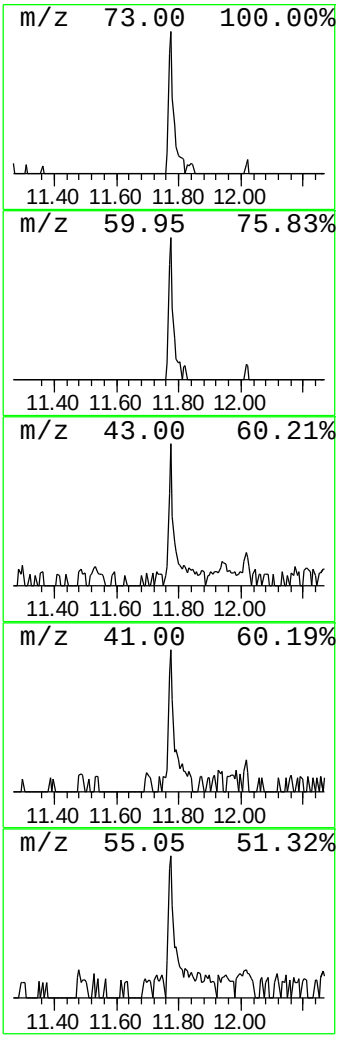
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.13 ng	67719	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	52
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	4-Chloropyridin-3-sulfonamide	192	C5H5ClN2O2S	1000306-78-8	22
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	11





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Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

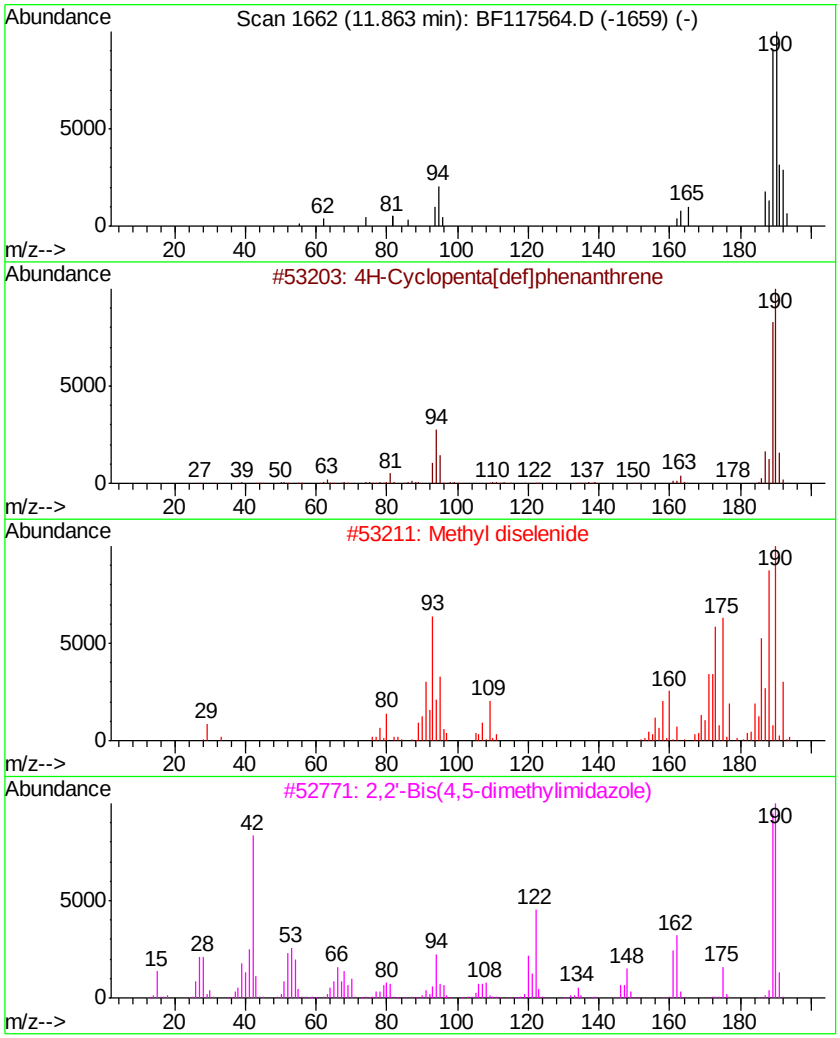
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

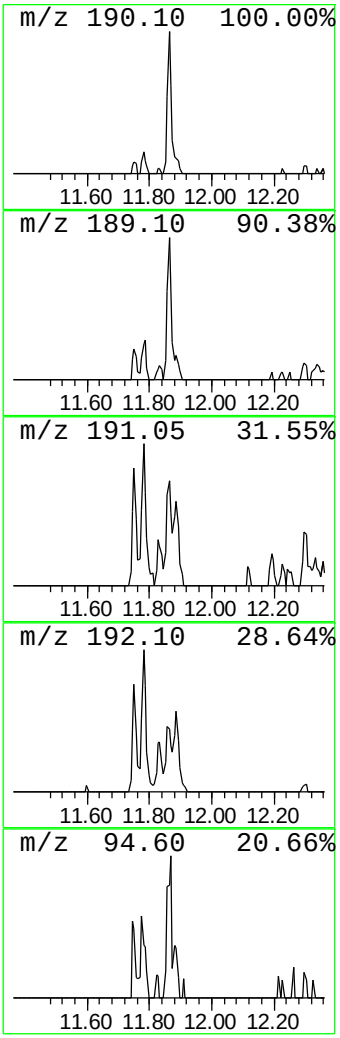
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.58 ng	34000	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	Methyl diselenide	190	C2H6Se2	007101-31-7	38
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	33
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	22





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TIC Library : C:\DATABASE\NIST11.L
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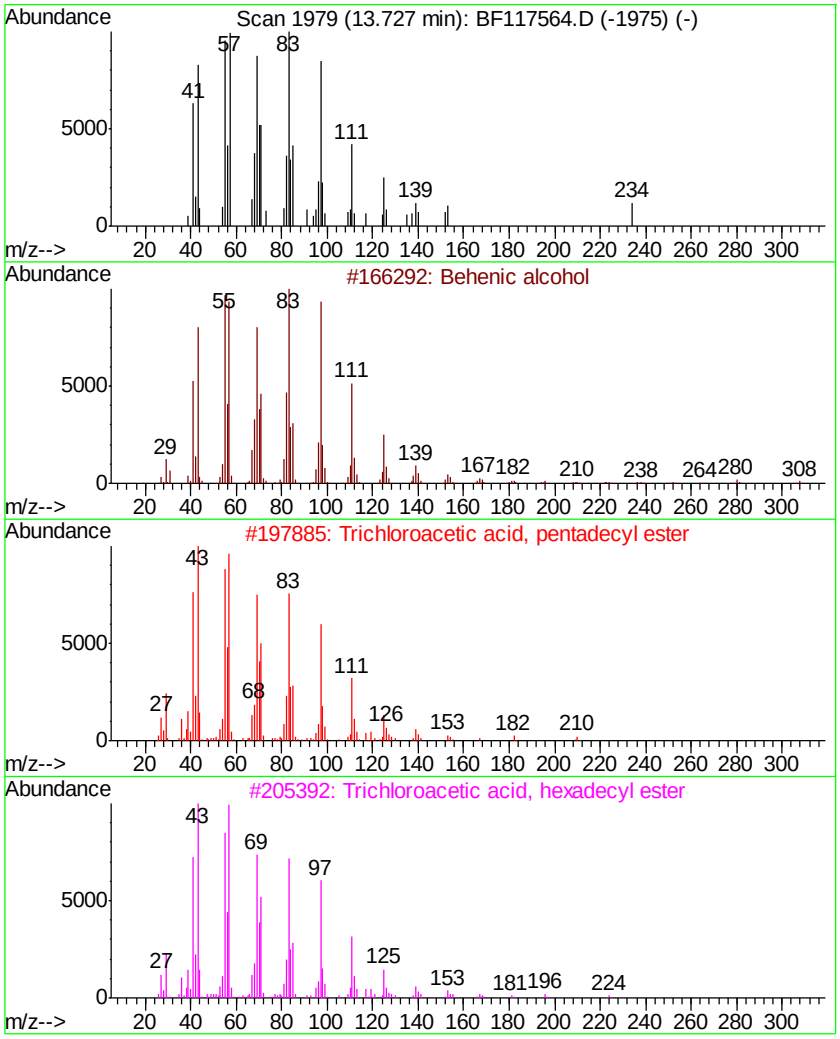
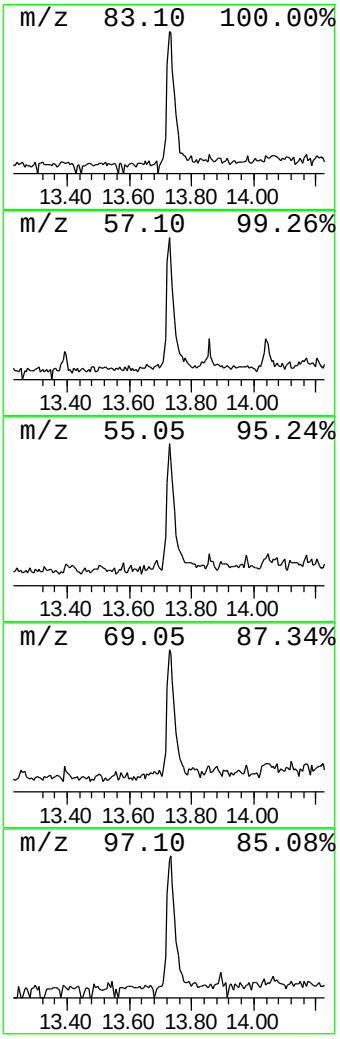
Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.36 ng	147506	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





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Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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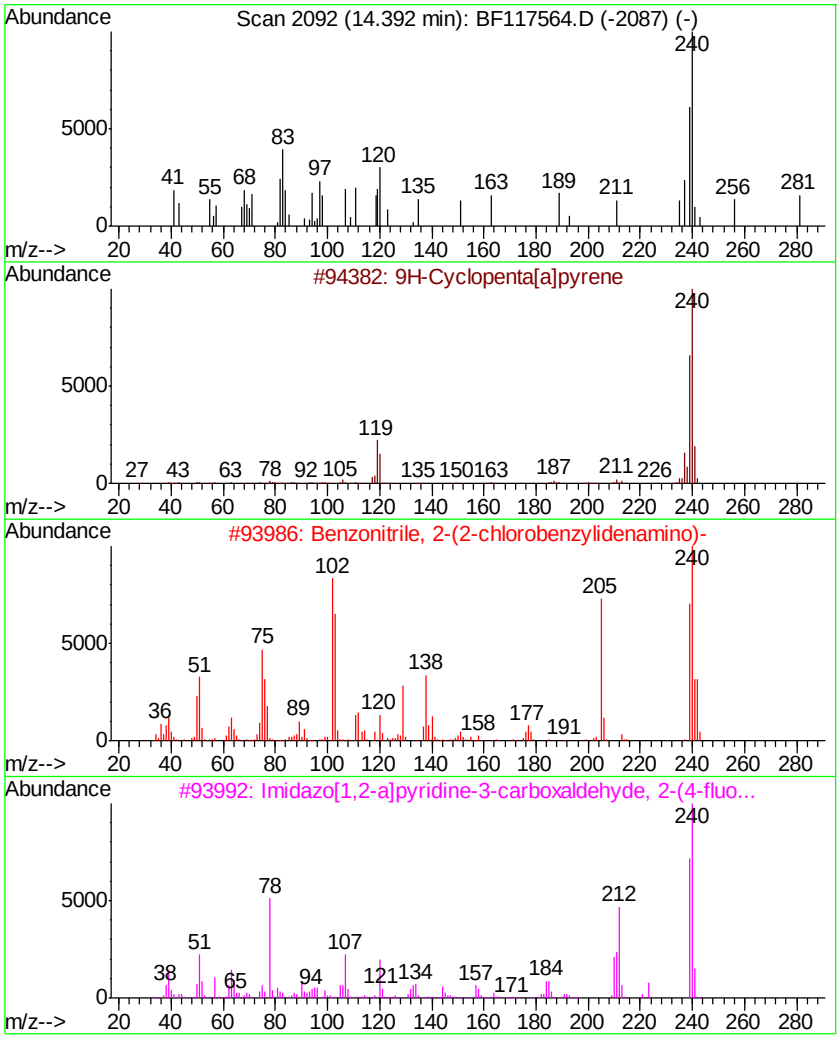
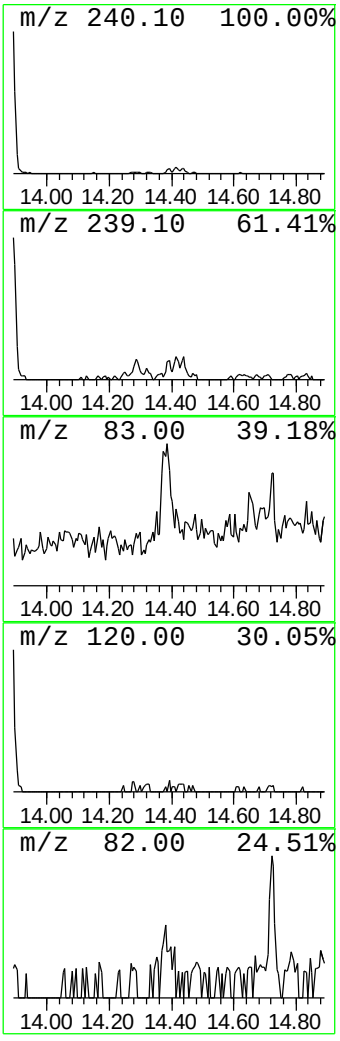
****

Peak Number 6 unknown14.39 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.07 ng	41544	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Cyclopenta[a]pyrene	240	C19H12	050861-05-7	28
2	Benzonitrile, 2-(2-chlorobenzyli...	240	C14H9ClN2	104830-19-5	25
3	Imidazo[1,2-a]pyridine-3-carboxa...	240	C14H9FN2O	1000351-44-5	25
4	1-Methyl-3-phenylsulfanyl-1H-indole	239	C15H13NS	1000322-52-6	23
5	1,2,4-Triazolo[4,3-a]pyrimidin-5...	240	C13H12N4O	1000268-26-5	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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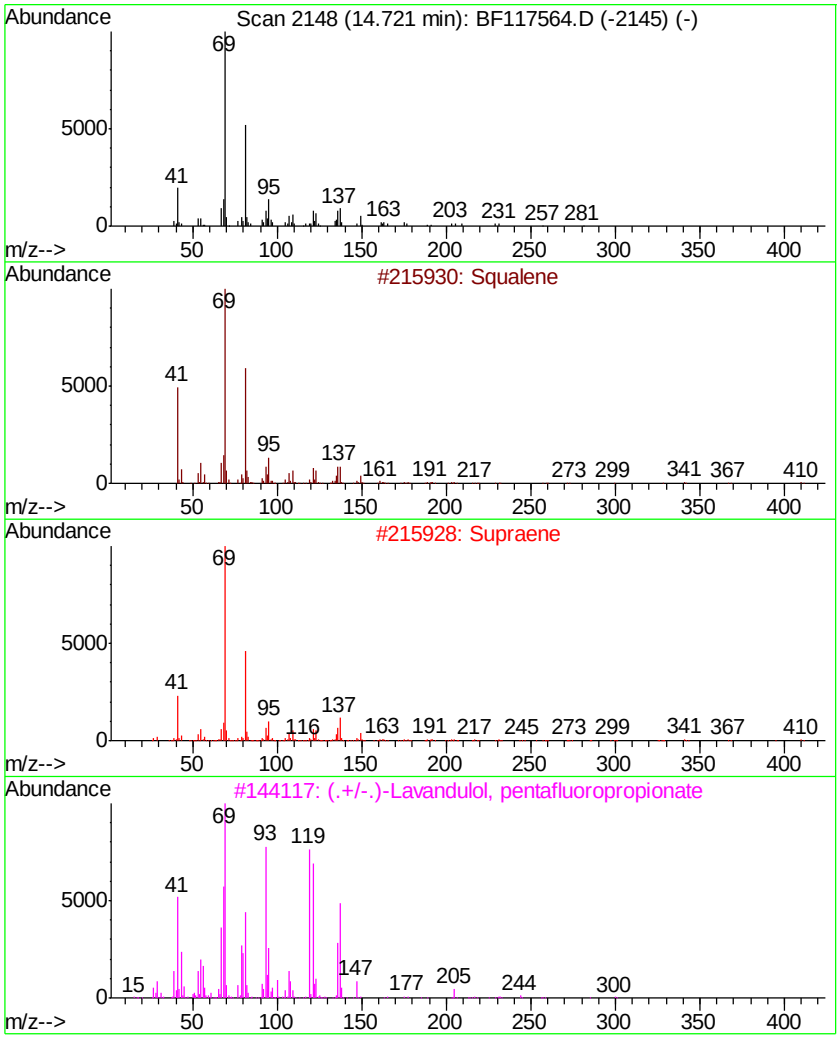
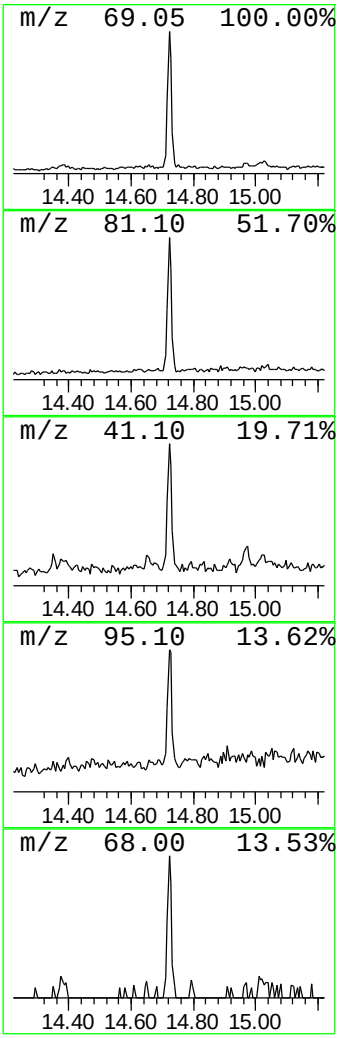
Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	9.93 ng	106734	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72





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TIC Integration Parameters: LSCINT.P

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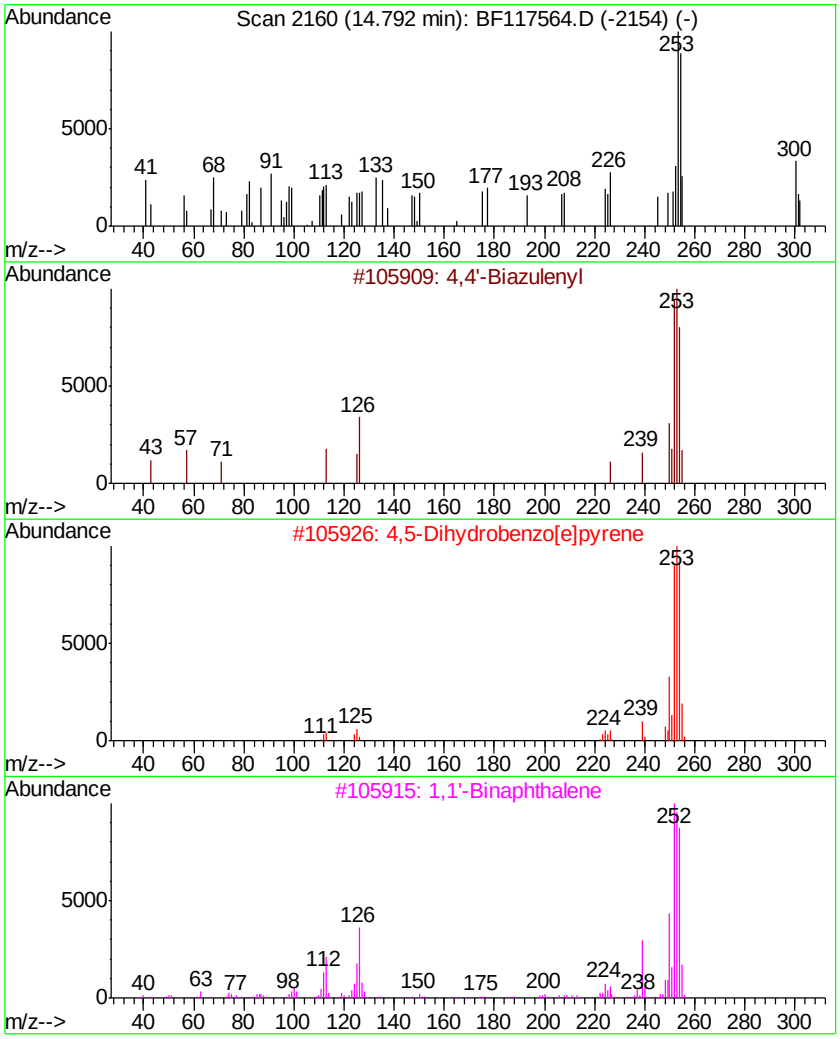
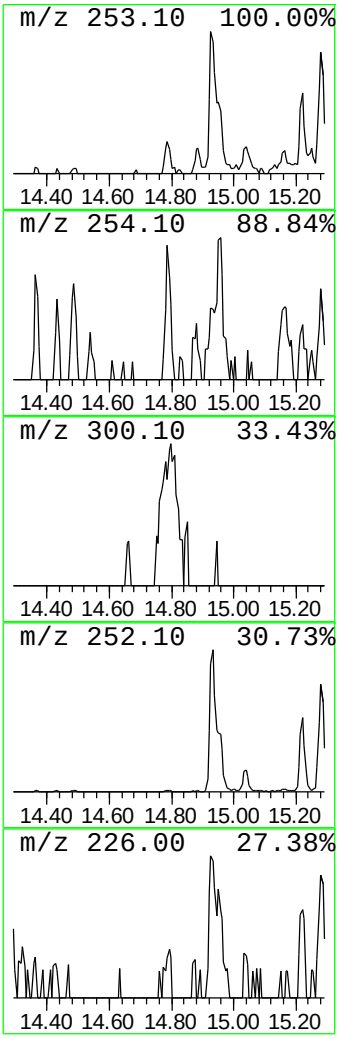
Peak Number 8 4,4'-Biazulenyl Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.07 ng	32955	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Biazulenyl	254	C20H14	094053-54-0	70
2	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	64
3	1,1'-Binaphthalene	254	C20H14	000604-53-5	58
4	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	53
5	4,6'-Biazulenyl	254	C20H14	094154-49-1	52





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Data File : BF117564.D
Acq On : 28 Oct 2019 16:31
Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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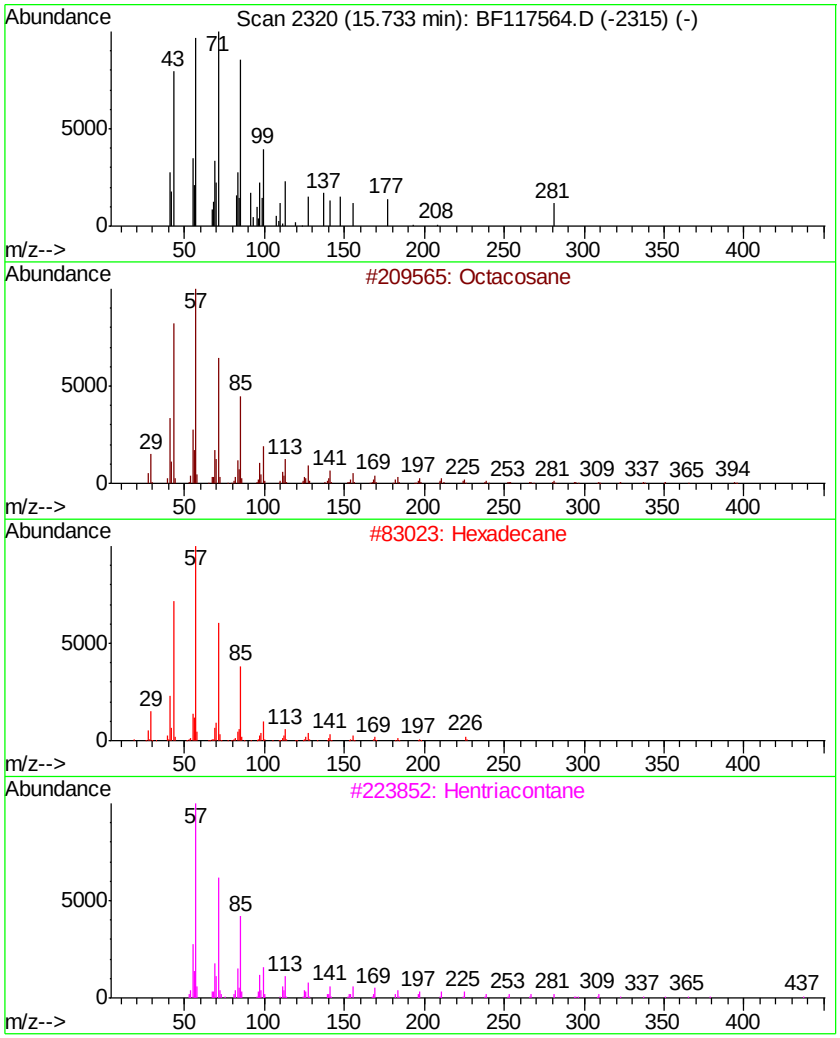
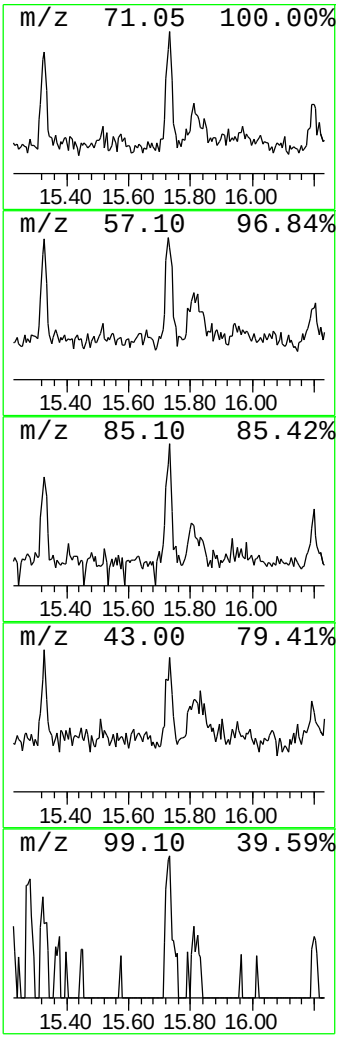
Peak Number 11 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.71 ng	29180	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Hexadecane	226	C16H34	000544-76-3	72
3	Hentriacontane	437	C31H64	000630-04-6	72
4	2-methyltetracosane	352	C25H52	1000376-72-6	72
5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117564.D
Acq On : 28 Oct 2019 16:31
Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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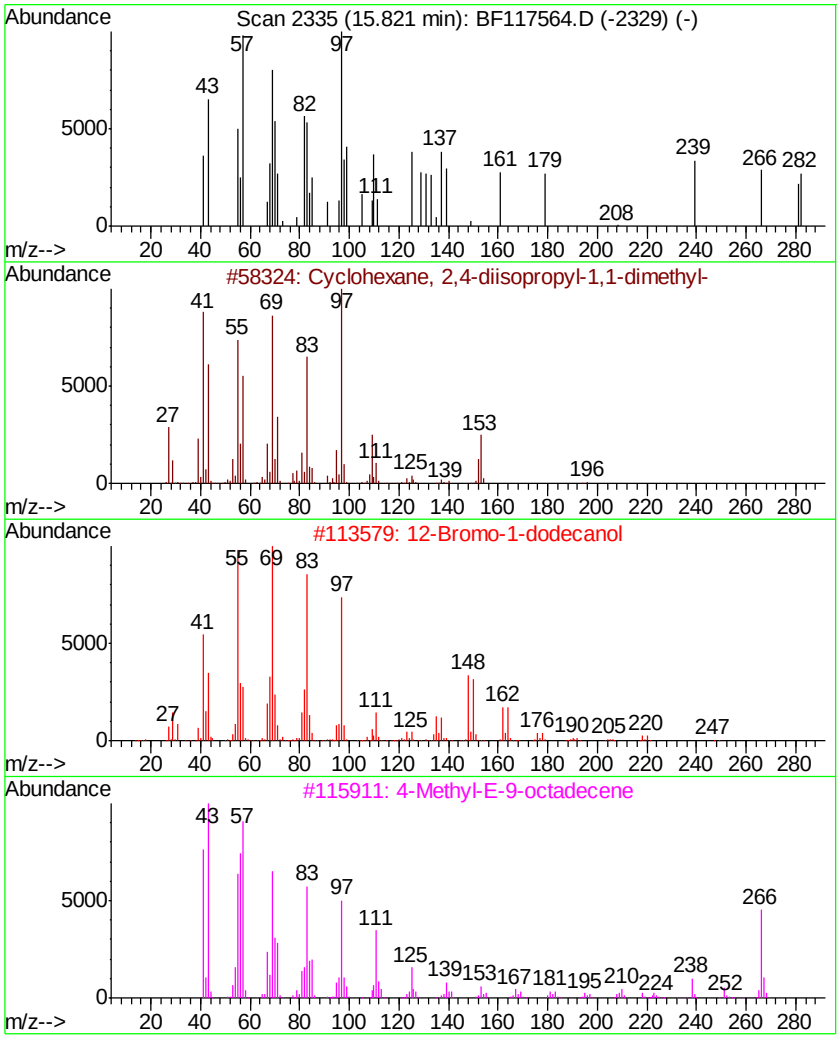
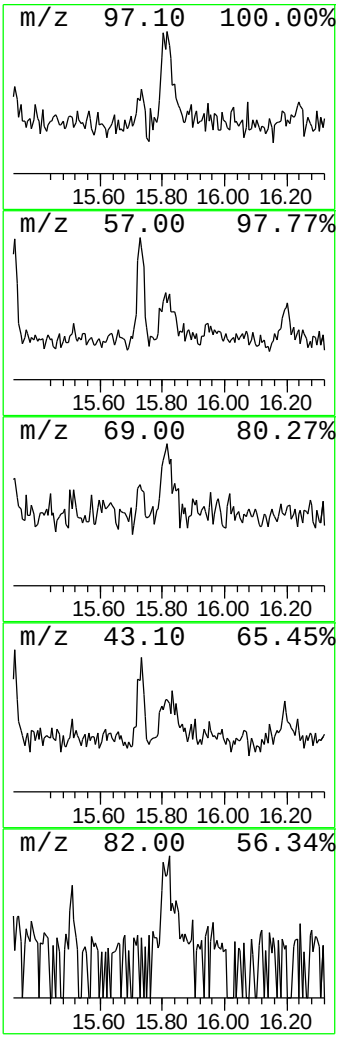
Peak Number 12 unknown15.82 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.89 ng	31071	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	43
2	12-Bromo-1-dodecanol	264	C12H25BrO	003344-77-2	43
3	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	25
4	6-Methyl-1,5-diazabicyclo[3.1.0]...	98	C5H10N2	100463-00-1	25
5	1-Tetradecanol	214	C14H30O	000112-72-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102819\
Data File : BF117564.D
Acq On : 28 Oct 2019 16:31
Operator : JU
Sample : K5501-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 187-30-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	79.1	ng	840931	1	6.73	212668	20.0
n-Hexadecanoic acid	11.77	5.1	ng	67719	4	11.24	263871	20.0
4H-Cyclopenta[def...	11.86	2.6	ng	34000	4	11.24	263871	20.0
Behenic alcohol	13.73	7.4	ng	147506	5	13.89	400916	20.0
unknown14.39	14.39	2.1	ng	41544	5	13.89	400916	20.0
Squalene	14.72	9.9	ng	106734	6	15.34	214983	20.0
4,4'-Biazulenyl	14.79	3.1	ng	32955	6	15.34	214983	20.0
Octacosane	15.73	2.7	ng	29180	6	15.34	214983	20.0
unknown15.82	15.82	2.9	ng	31071	6	15.34	214983	20.0