LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117943.D
Acq On : 23 Nov 2019 2:46
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

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-BF111319.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	2.204	14	20	32	rVB	831604	1077672	28.84%	2.460%
2	5.122	506	516	525	rBV	546179	671154	17.96%	1.532%
3	5.522	579	584	587	rBV	3045268	3112162	83.28%	7.105%
4	6.528	749	755	758	rBV	3262454	3352384	89.71%	7.654%
5	6.669	775	779	783	rBV	3588485	3566856	95.45%	8.144%
6	6.904	815	819	822	rBV	1317506	1052329	28.16%	2.403%
7	7.063	841	846	849	rBV	2891075	2673084	71.53%	6.103%
8	7.463	909	914	917	rBV	2205916	2084423	55.78%	4.759%
9	8.192	1033	1038	1041	rBV	1413779	1310434	35.07%	2.992%
10	9.269	1216	1221	1224	rBV	4358443	3736921	100.00%	8.532%
11	9.663	1284	1288	1295	rVB	584614	514682	13.77%	1.175%
12	9.810	1310	1313	1317	rBV	67105	57925	1.55%	0.132%
13	9.951	1331	1337	1340	rBV	1818515	1551758	41.53%	3.543%
14	9.986	1340	1343	1346	rVB	134339	118799	3.18%	0.271%
15	10.157	1368	1372	1376	rVB	63711	61127	1.64%	0.140%
16	10.498	1427	1430	1436	rVB	110850	105200	2.82%	0.240%
17	10.739	1467	1471	1475	rBV	2262525	2198004	58.82%	5.018%
18	11.339	1569	1573	1578	rVB	58747	66326	1.77%	0.151%
19	11.445	1587	1591	1593	rBV	1645079	1435612	38.42%	3.278%
20	11.469	1593	1595	1598	rVV	1127165	830534	22.23%	1.896%
21	11.516	1598	1603	1607	rVB	254591	257917	6.90%	0.589%
22	11.674	1624	1630	1633	rBV	68773	78565	2.10%	0.179%
23	11.898	1664	1668	1672	rBV	139020	171707	4.59%	0.392%
24	11.969	1677	1680	1687	rVV2	585637	670642	17.95%	1.531%
25	12.022	1687	1689	1692	rVV	64205	60691	1.62%	0.139%
26	12.063	1692	1696	1698	rVV2	214132	232182	6.21%	0.530%
27	12.080	1698	1699	1702	rVB	86549	61727	1.65%	0.141%
28	12.245	1724	1727	1729	rBV	76290	69858	1.87%	0.159%
29	12.263	1729	1730	1734	rVB2	54837	48229	1.29%	0.110%
30	12.498	1767	1770	1773	rBV	95833	95046	2.54%	0.217%
31	12.533	1773	1776	1778	rVV2	57066	61160	1.64%	0.140%
32	12.580	1782	1784	1789	rVB2	62012	67379	1.80%	0.154%
33	12.663	1794	1798	1801	rBV	1416659	1153485	30.87%	2.634%
34	12.757	1811	1814	1817	rBV	158676	164329	4.40%	0.375%

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Integrator: RTE
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.816	1821	1824	1831	rVB4	54930	86514	2.32%	0.198%
36	12.892	1831	1837	1843	rBV	970799	1025944	27.45%	2.342%
37	12.939	1843	1845	1850	rVB2	47107	63234	1.69%	0.144%
38	13.033	1857	1861	1864	rVB	2806387	2366421	63.33%	5.403%
39	13.104	1869	1873	1878	rBV3	65586	114735	3.07%	0.262%
40	13.198	1885	1889	1890	rBV4	49200	58249	1.56%	0.133%
41	13.221	1890	1893	1895	rVB	139758	120833	3.23%	0.276%
42	13.286	1902	1904	1906	rVB2	109689	78874	2.11%	0.180%
43	13.321	1906	1910	1913	rBV2	86708	89402	2.39%	0.204%
44	13.416	1924	1926	1929	rBV	54929	44880	1.20%	0.102%
45	13.451	1929	1932	1935	rBV	67786	68769	1.84%	0.157%
46	13.604	1954	1958	1960	rBV5	40286	54422	1.46%	0.124%
47	13.727	1976	1979	1983	rVB	72529	73055	1.95%	0.167%
48	13.839	1994	1998	2001	rBV2	80342	101705	2.72%	0.232%
49	13.868	2001	2003	2005	rVV	80932	69132	1.85%	0.158%
50	13.892	2005	2007	2011	rVV2	86104	104713	2.80%	0.239%
51	13.933	2011	2014	2021	rVB2	197573	249376	6.67%	0.569%
52	14.092	2036	2041	2044	rBV2	1276050	1625228	43.49%	3.711%
53	14.115	2044	2045	2052	rVB	505793	374691	10.03%	0.855%
54	14.198	2057	2059	2061	rVB	104218	74041	1.98%	0.169%
55	14.239	2063	2066	2067	rBV	45314	51207	1.37%	0.117%
56	14.480	2104	2107	2109	rVB	103882	96306	2.58%	0.220%
57	14.515	2109	2113	2116	rVV2	71143	81015	2.17%	0.185%
58	14.563	2117	2121	2122	rVV4	79894	114954	3.08%	0.262%
59	14.604	2126	2128	2130	rVV	78305	77589	2.08%	0.177%
60	14.627	2130	2132	2136	rVB	66610	57052	1.53%	0.130%
61	14.874	2171	2174	2177	rBV	66540	69981	1.87%	0.160%
62	14.957	2185	2188	2191	rBV2	94632	96802	2.59%	0.221%
63	15.151	2216	2221	2224	rBV	401071	620055	16.59%	1.416%
64	15.227	2231	2234	2237	rBV	59111	55872	1.50%	0.128%
65	15.262	2237	2240	2243	rBV	96764	97348	2.61%	0.222%
66	15.462	2270	2274	2280	rVB	230599	325992	8.72%	0.744%
67	15.527	2281	2285	2291	rVB	381102	493156	13.20%	1.126%
68	15.598	2292	2297	2300	rBV	849962	1061834	28.41%	2.424%
69	15.627	2300	2302	2308	rVB2	161967	200838	5.37%	0.459%
70	17.115	2549	2555	2563	rBV2	181251	364173	9.75%	0.831%
71	17.580	2628	2634	2644	rVB	153177	321166	8.59%	0.733%

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Integrator: RTE
Smoothing : ON Filtering: 5
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 43799861

LSC Report - Integrated Chromatogram

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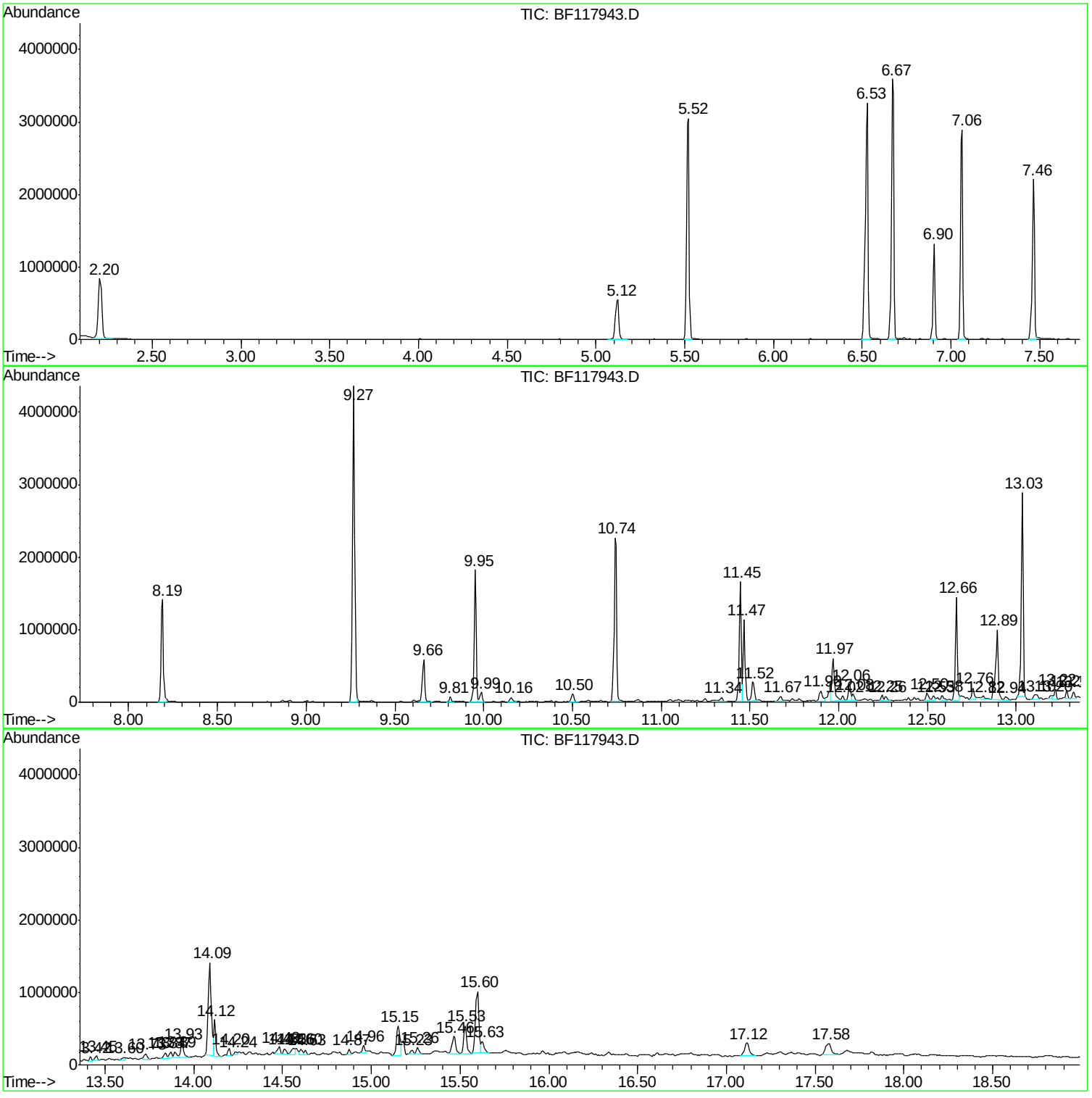
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112219\
Data File : BF117943.D
Acq On : 23 Nov 2019 2:46
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Sample : K5671-11
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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

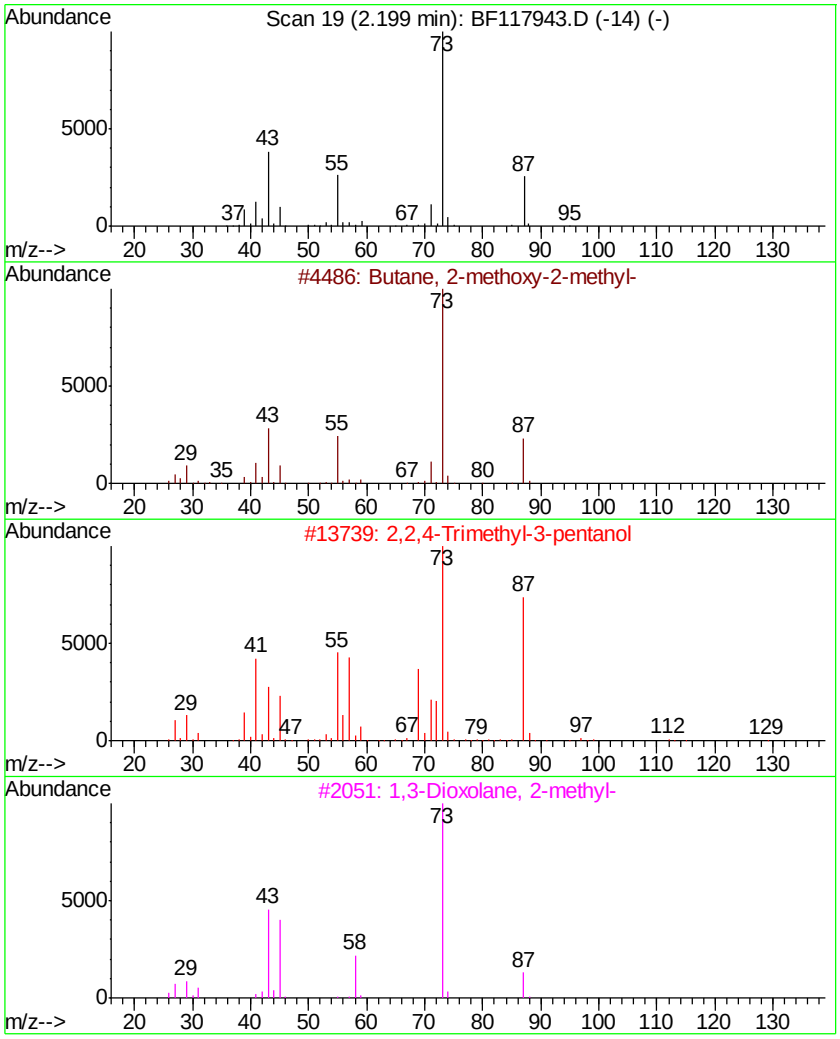
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

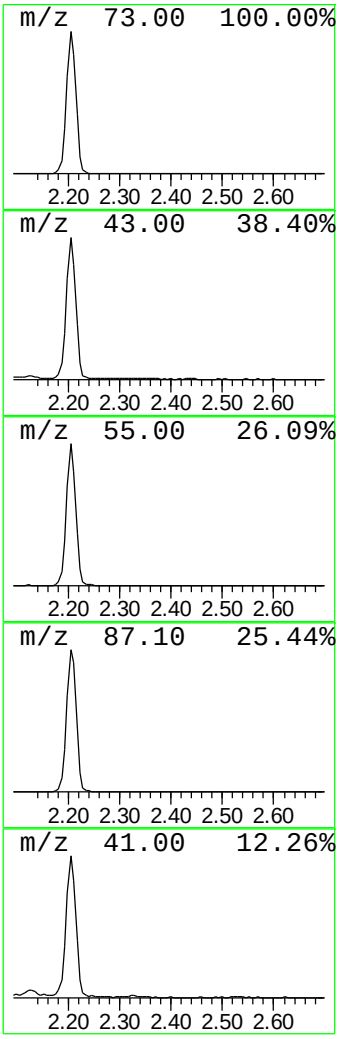
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	20.48 ng	1077670	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

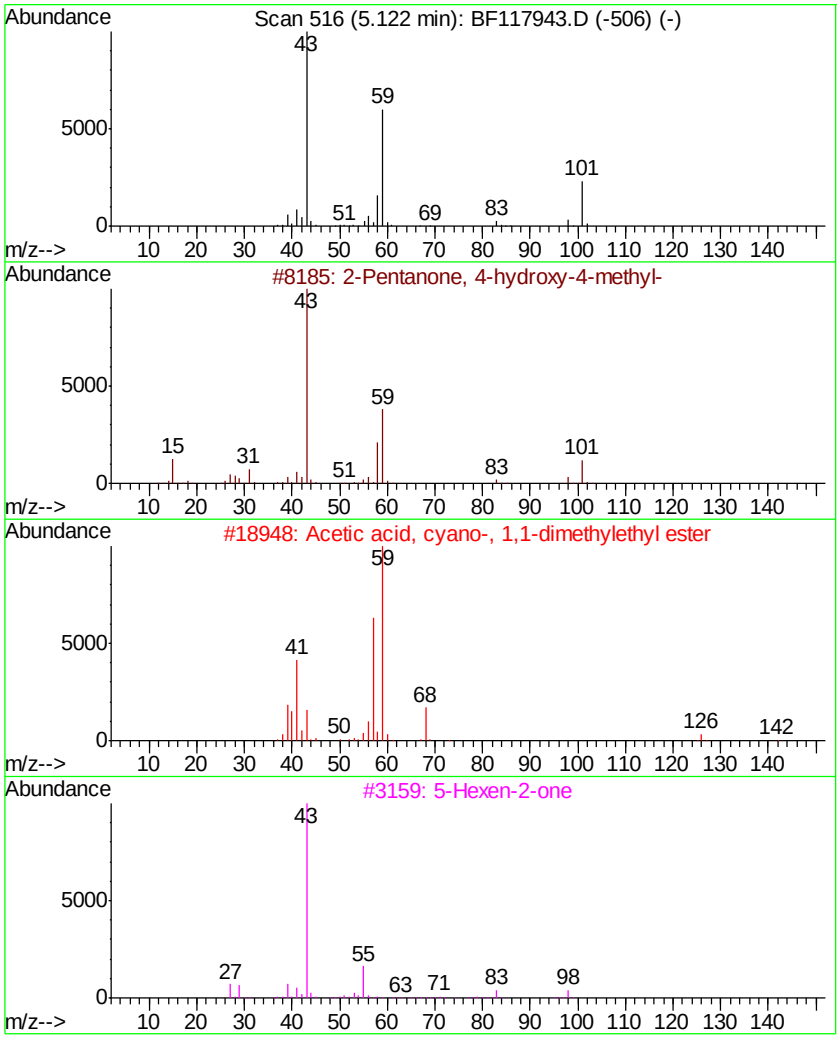
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

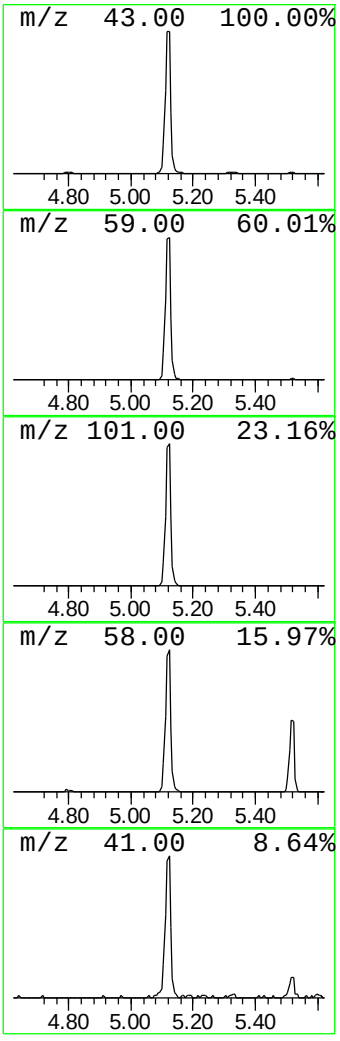
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.76 ng	671154	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

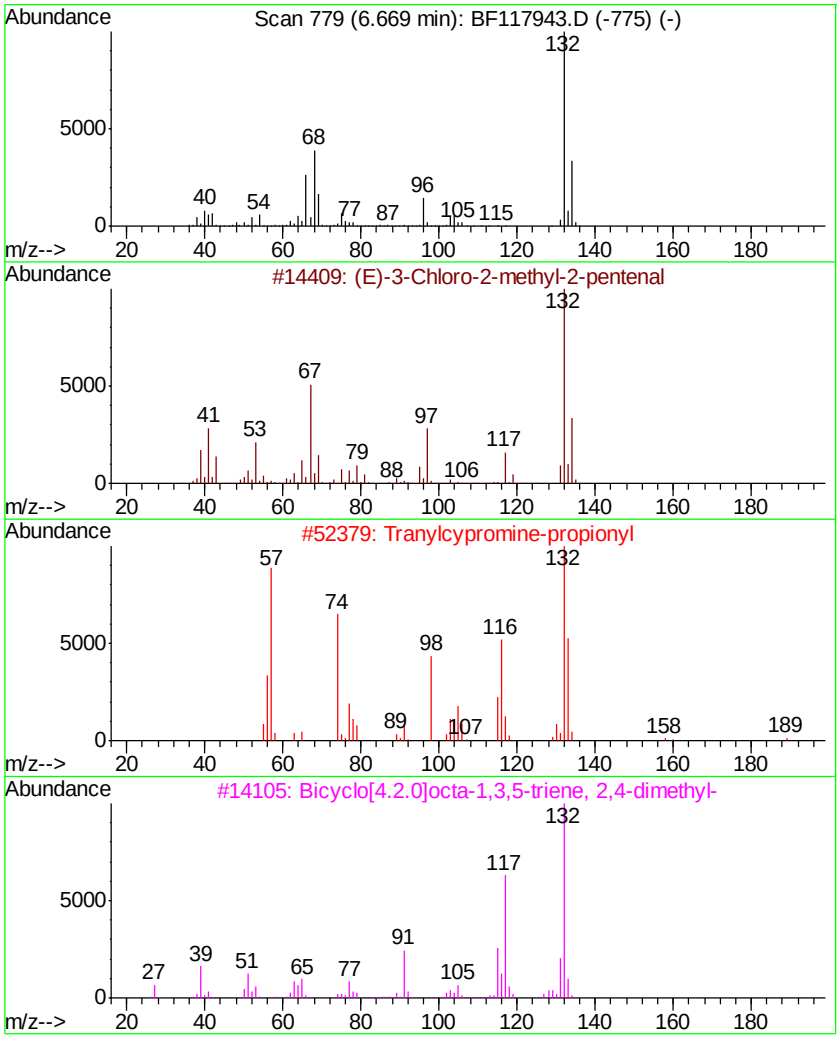
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

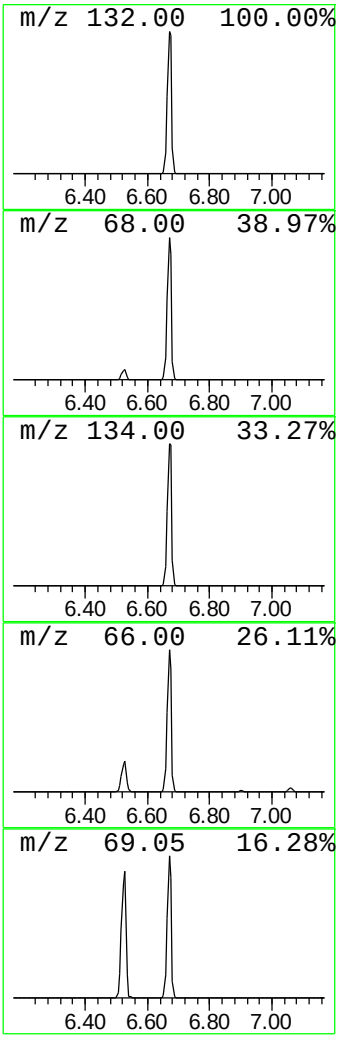
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	67.79 ng	3566860	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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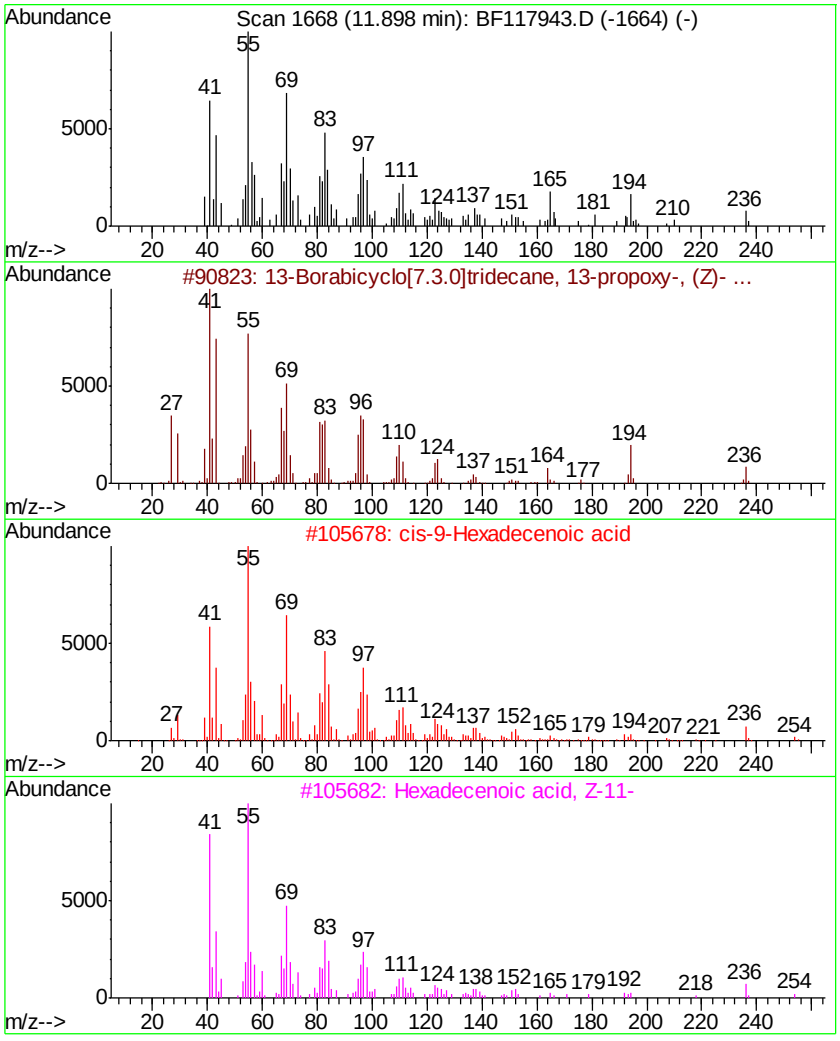
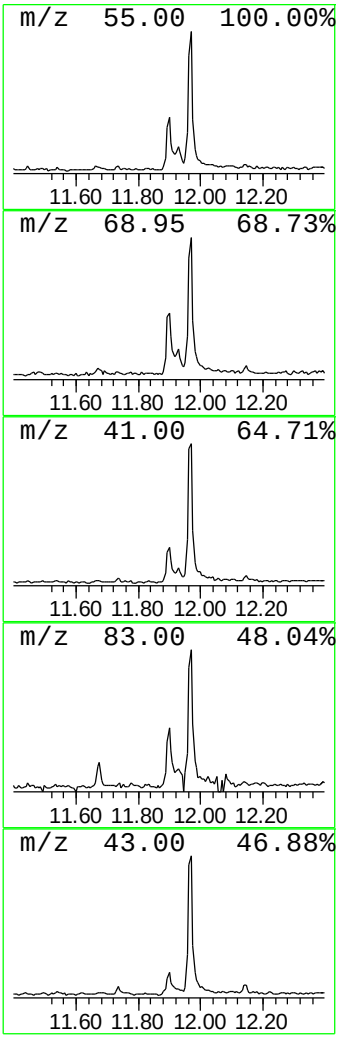
****

Peak Number 5 13-Borabicyclo[7.3.0]tridec... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.39 ng	171707	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	94
2	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	93
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90
4	Palmitoleic acid	254	C16H30O2	000373-49-9	81
5	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	68





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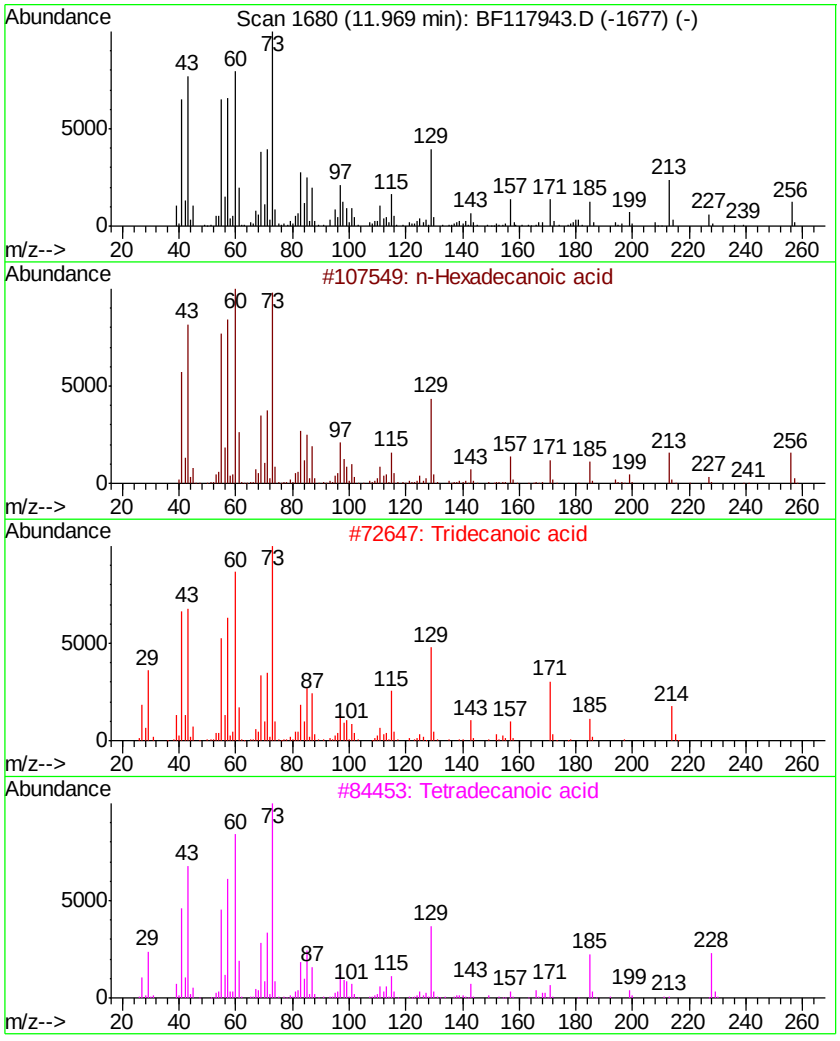
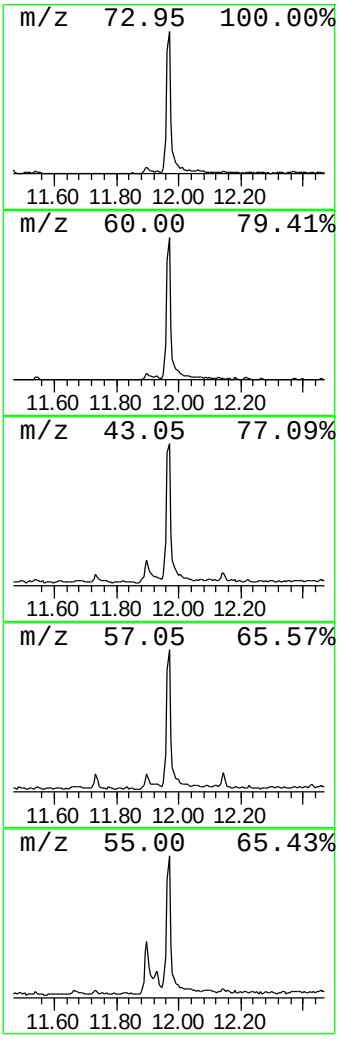
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	9.34 ng	670642	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

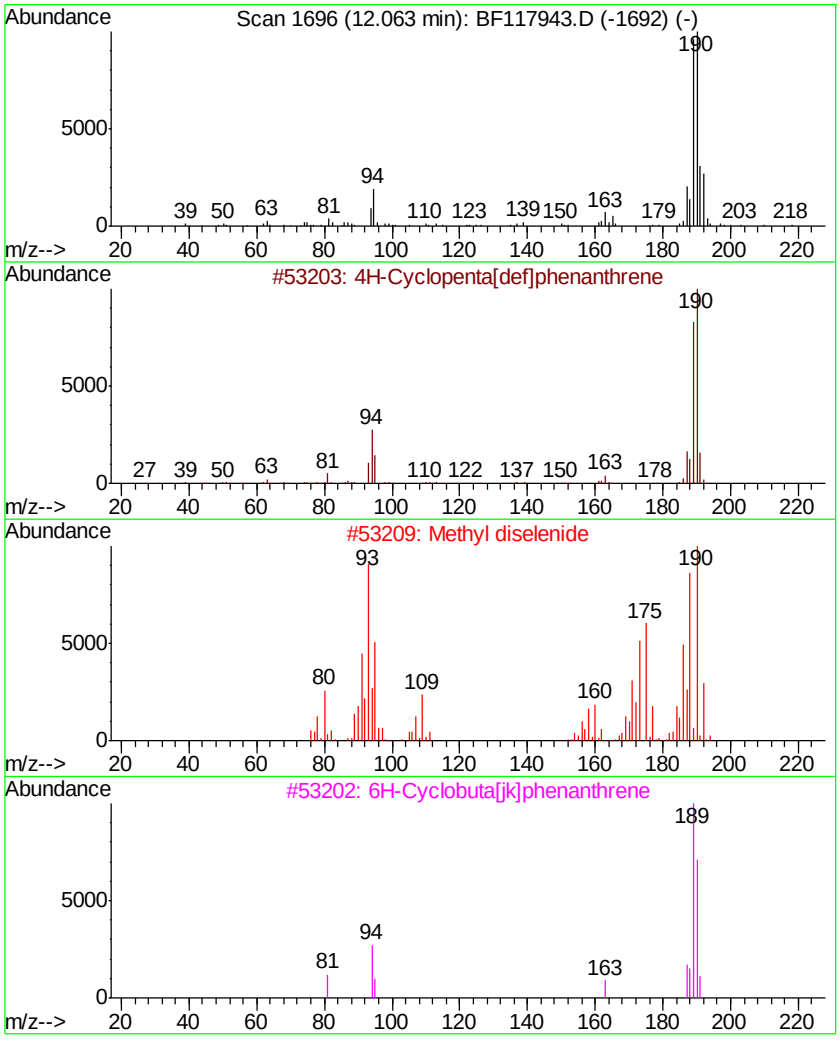
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

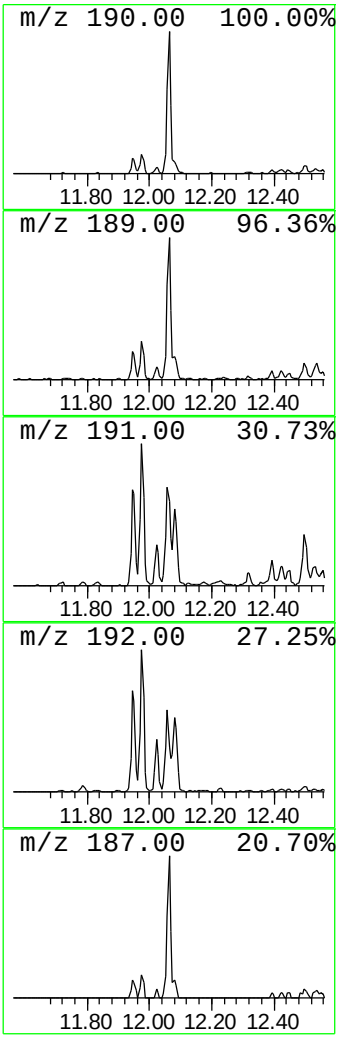
****

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	3.23 ng	232182	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





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Instrument : BNA_F
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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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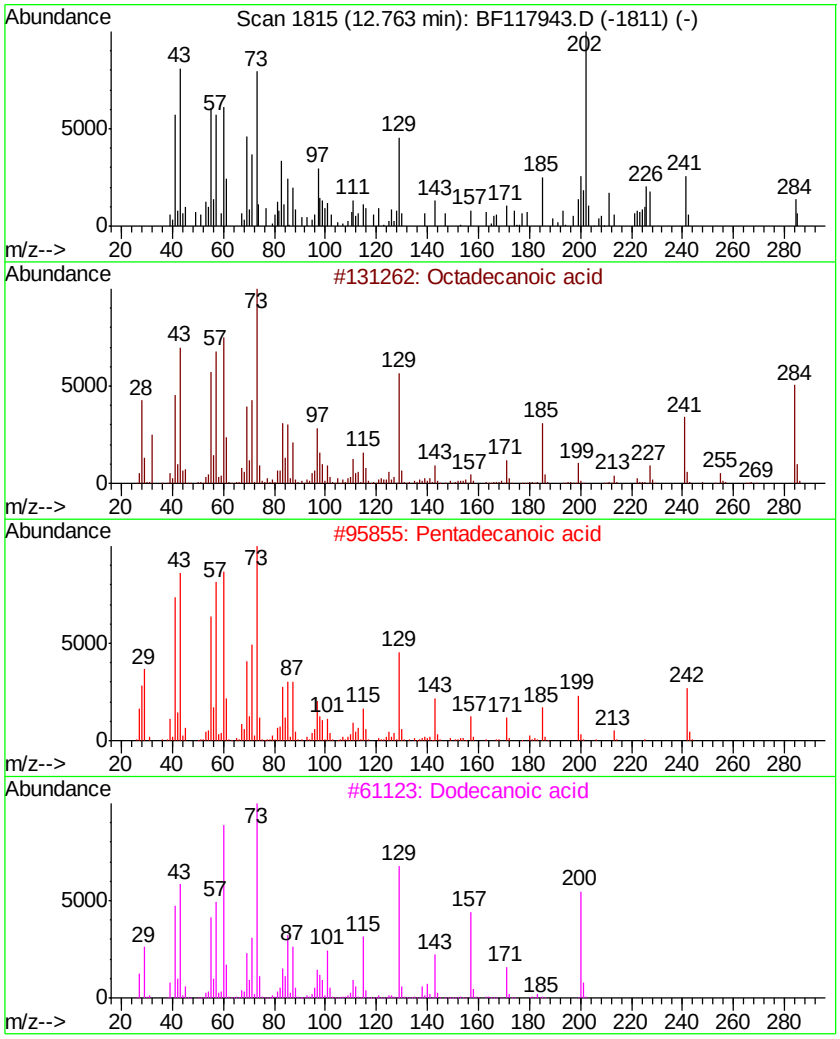
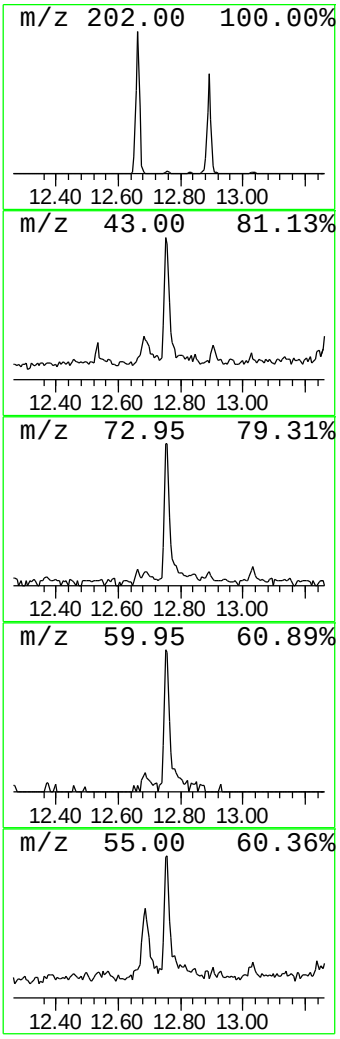
Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.29 ng	164329	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	46
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	45
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Data File : BF117943.D
Acq On : 23 Nov 2019 2:46
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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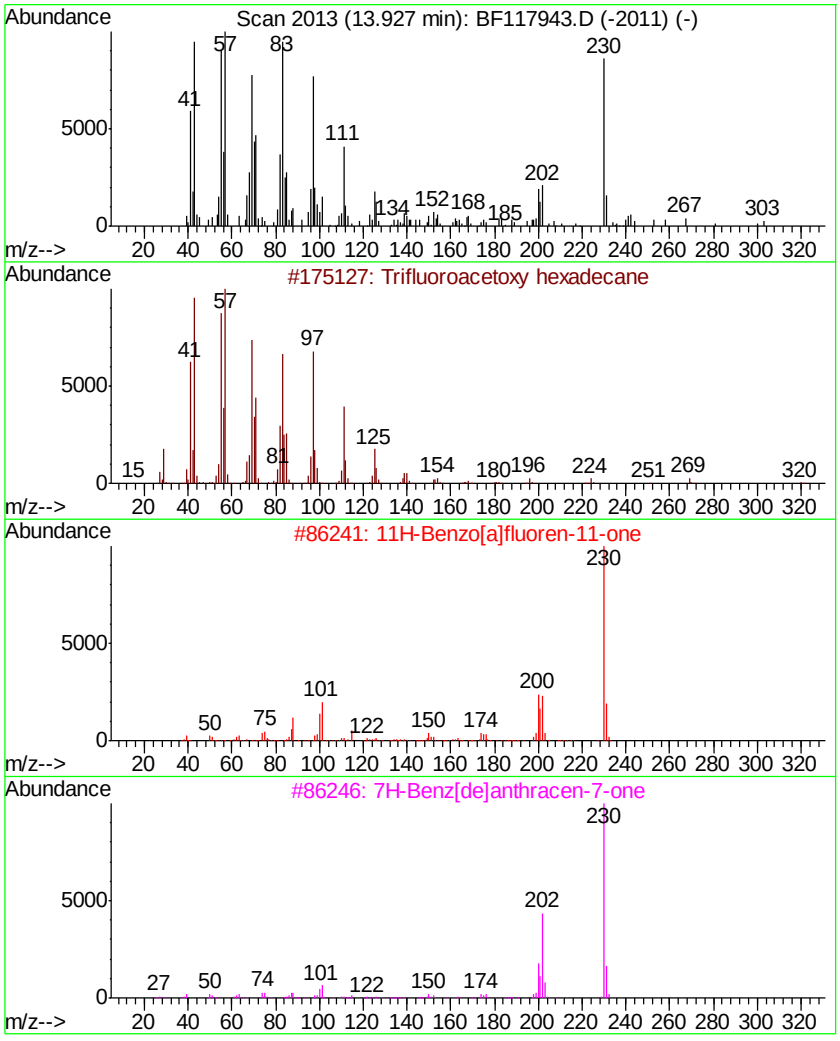
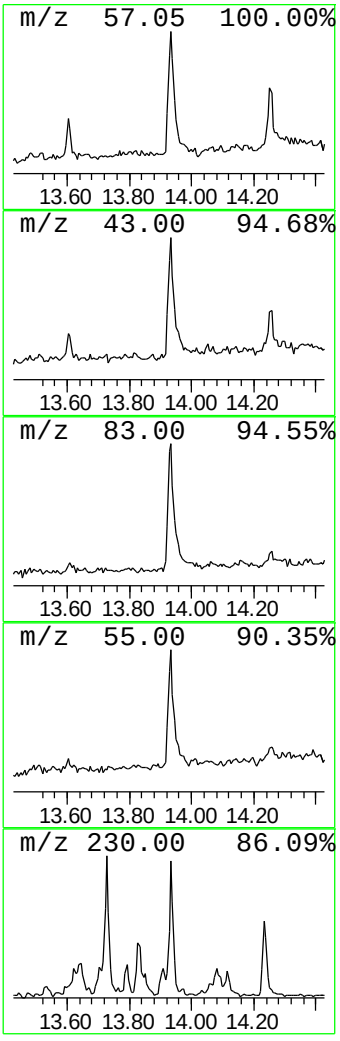
Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.07 ng	249376	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83
2	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	64
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	46
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	46





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112219\
Data File : BF117943.D
Acq On : 23 Nov 2019 2:46
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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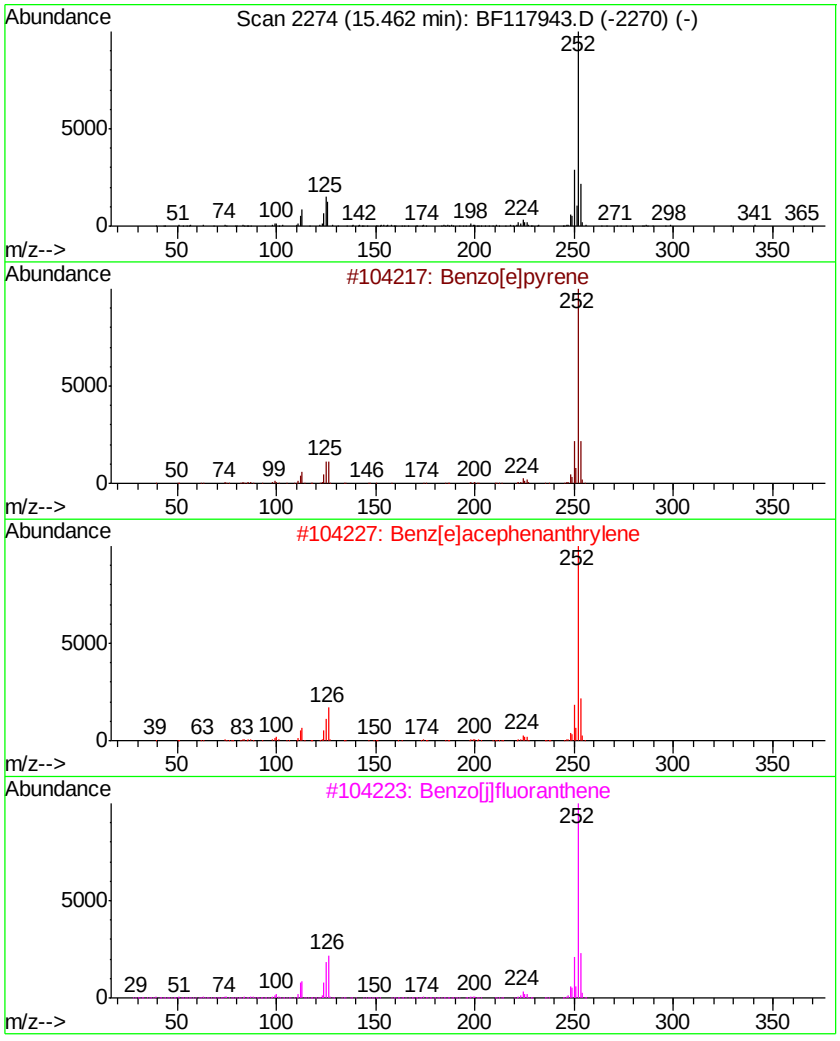
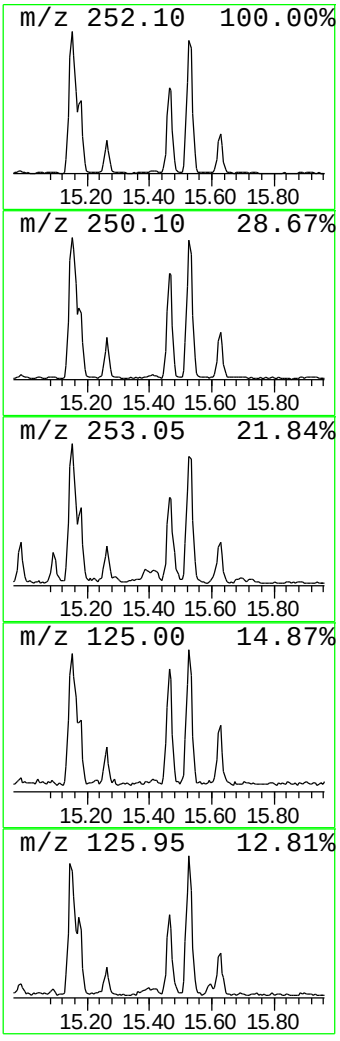
Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	6.14 ng	325992	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112219\
Data File : BF117943.D
Acq On : 23 Nov 2019 2:46
Operator : JU
Sample : K5671-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-112119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.20	20.5	ng	1077670	1	6.90	1052330	20.0
2-Pentanone, 4-hy...	5.12	12.8	ng	671154	1	6.90	1052330	20.0
unknown6.67	6.67	67.8	ng	3566860	1	6.90	1052330	20.0
13-Borabicyclo[7....	11.90	2.4	ng	171707	4	11.45	1435610	20.0
n-Hexadecanoic acid	11.97	9.3	ng	670642	4	11.45	1435610	20.0
4H-Cyclopenta[def...	12.06	3.2	ng	232182	4	11.45	1435610	20.0
Octadecanoic acid	12.76	2.3	ng	164329	4	11.45	1435610	20.0
Trifluoroacetoxy ...	13.93	3.1	ng	249376	5	14.09	1625230	20.0
Benzo[e]pyrene	15.46	6.1	ng	325992	6	15.60	1061830	20.0