LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117673.D
Acq On : 31 Oct 2019 22:01
Operator : JU
Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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	4.910	477	480	491	rBV	24430	42267	11.36%	0.873%
2	5.363	554	557	580	rBV	131365	280357	75.35%	5.788%
3	5.551	586	589	599	rVB	17857	23048	6.19%	0.476%
4	6.393	729	732	748	rBV	156228	321726	86.46%	6.642%
5	6.510	748	752	766	rVB	280344	372092	100.00%	7.682%
6	6.728	786	789	799	rBV	196056	185420	49.83%	3.828%
7	6.881	812	815	828	rBV	245671	264810	71.17%	5.467%
8	7.304	883	887	904	rBV	91131	186380	50.09%	3.848%
9	8.010	1004	1007	1034	rBV	155619	243138	65.34%	5.020%
10	8.610	1106	1109	1116	rBB2	8884	10497	2.82%	0.217%
11	9.081	1186	1189	1202	rBV	280371	326404	87.72%	6.739%
12	9.486	1255	1258	1266	rBV	44072	52017	13.98%	1.074%
13	9.628	1280	1282	1285	rBV	4359	4247	1.14%	0.088%
14	9.763	1301	1305	1318	rBV	233169	253081	68.02%	5.225%
15	10.022	1344	1349	1355	rVB2	3213	5865	1.58%	0.121%
16	10.563	1437	1441	1455	rBV	110628	140216	37.68%	2.895%
17	10.680	1459	1461	1467	rVV	5387	5797	1.56%	0.120%
18	10.733	1467	1470	1473	rVV	10362	9879	2.65%	0.204%
19	10.769	1473	1476	1479	rVV3	9213	12651	3.40%	0.261%
20	10.798	1479	1481	1484	rVV2	9074	10023	2.69%	0.207%
21	10.822	1484	1485	1489	rVB	5183	4851	1.30%	0.100%
22	10.875	1489	1494	1497	rBV2	3951	8721	2.34%	0.180%
23	10.910	1497	1500	1504	rVV2	7309	9346	2.51%	0.193%
24	10.951	1504	1507	1509	rVV	8915	8707	2.34%	0.180%
25	10.986	1512	1513	1517	rVB	4944	4300	1.16%	0.089%
26	11.104	1531	1533	1536	rVB	8705	7134	1.92%	0.147%
27	11.251	1554	1558	1561	rBV	193636	196159	52.72%	4.050%
28	11.275	1561	1562	1568	rVV	60255	56621	15.22%	1.169%
29	11.333	1568	1572	1577	rVB	11292	13167	3.54%	0.272%
30	11.404	1582	1584	1590	rVB3	2894	3834	1.03%	0.079%
31	11.651	1621	1626	1634	rBV3	11788	12596	3.39%	0.260%
32	11.757	1638	1644	1645	rBV4	11842	13959	3.75%	0.288%
33	11.780	1645	1648	1650	rVV2	28124	39531	10.62%	0.816%
34	11.804	1650	1652	1655	rVV	38940	34090	9.16%	0.704%

LSC Area Percent Report

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Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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

35	11.839	1655	1658	1660	rVV3	6220	7418	1.99%	0.153%
36	11.869	1660	1663	1666	rVV	18045	22565	6.06%	0.466%
37	11.892	1666	1667	1670	rVV2	8735	7562	2.03%	0.156%
38	12.051	1689	1694	1698	rBV3	5431	7863	2.11%	0.162%
39	12.104	1701	1703	1709	rVB4	5382	7647	2.06%	0.158%
40	12.204	1713	1720	1721	rBV3	7373	11116	2.99%	0.229%
41	12.269	1729	1731	1734	rVB2	3719	3738	1.00%	0.077%
42	12.304	1734	1737	1739	rBV2	11073	10697	2.87%	0.221%
43	12.327	1739	1741	1743	rBV2	4854	4866	1.31%	0.100%
44	12.410	1750	1755	1756	rBV5	3412	5073	1.36%	0.105%
45	12.439	1757	1760	1762	rVV3	8806	6827	1.83%	0.141%
46	12.469	1762	1765	1774	rVB	110900	108965	29.28%	2.250%
47	12.563	1779	1781	1785	rBV3	6841	10383	2.79%	0.214%
48	12.622	1788	1791	1798	rBV6	4777	7685	2.07%	0.159%
49	12.698	1798	1804	1808	rBV	108473	129414	34.78%	2.672%
50	12.827	1823	1826	1833	rVB	277012	252721	67.92%	5.218%
51	12.922	1838	1842	1845	rVB6	9996	14529	3.90%	0.300%
52	12.969	1847	1850	1852	rBV4	4308	4322	1.16%	0.089%
53	13.010	1852	1857	1858	rBV4	8934	12348	3.32%	0.255%
54	13.033	1858	1861	1862	rVV2	12256	13221	3.55%	0.273%
55	13.051	1862	1864	1869	rVV3	23086	26916	7.23%	0.556%
56	13.092	1869	1871	1874	rVB	8048	7041	1.89%	0.145%
57	13.133	1876	1878	1883	rBV3	8798	12320	3.31%	0.254%
58	13.221	1892	1893	1897	rVB3	11802	9808	2.64%	0.202%
59	13.257	1897	1899	1904	rBV4	9742	15604	4.19%	0.322%
60	13.298	1904	1906	1910	rVB3	10108	10318	2.77%	0.213%
61	13.392	1919	1922	1925	rBV	22745	18105	4.87%	0.374%
62	13.557	1948	1950	1953	rVB3	8132	5460	1.47%	0.113%
63	13.651	1964	1966	1968	rBV2	9227	8413	2.26%	0.174%
64	13.704	1973	1975	1976	rVV	10862	7522	2.02%	0.155%
65	13.727	1976	1979	1984	rVV2	43846	70270	18.89%	1.451%
66	13.769	1984	1986	1991	rVB2	23035	23030	6.19%	0.475%
67	13.857	1998	2001	2003	rBV	24469	20016	5.38%	0.413%
68	13.898	2003	2008	2011	rVV2	204028	251321	67.54%	5.189%
69	13.921	2011	2012	2016	rVB	51600	47890	12.87%	0.989%
70	14.010	2024	2027	2028	rBV2	9702	8628	2.32%	0.178%
71	14.039	2029	2032	2035	rVV2	22424	20321	5.46%	0.420%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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72	14.345	2081	2084	2086	rBV2	21519	21562	5.79%	0.445%
73	14.468	2103	2105	2106	rBV2	11117	7045	1.89%	0.145%
74	14.639	2132	2134	2138	rVB2	33802	29786	8.01%	0.615%
75	14.933	2180	2184	2186	rBV	41780	58973	15.85%	1.218%
76	14.957	2186	2188	2193	rVB	61630	60522	16.27%	1.250%
77	15.221	2230	2233	2236	rBV	31497	36972	9.94%	0.763%
78	15.286	2241	2244	2245	rBV	22750	25546	6.87%	0.527%
79	15.339	2250	2253	2263	rVB	107227	168650	45.32%	3.482%
80	15.715	2314	2317	2320	rVB2	23753	26978	7.25%	0.557%
81	16.174	2393	2395	2397	rBV3	12012	12900	3.47%	0.266%
82	16.662	2476	2478	2479	rBV2	6915	6014	1.62%	0.124%
83	17.992	2702	2704	2707	rBV4	4496	4941	1.33%	0.102%
84	18.092	2719	2721	2725	rBV5	4215	4885	1.31%	0.101%
85	18.180	2734	2736	2737	rBV2	4630	3967	1.07%	0.082%

Sum of corrected areas: 4843615

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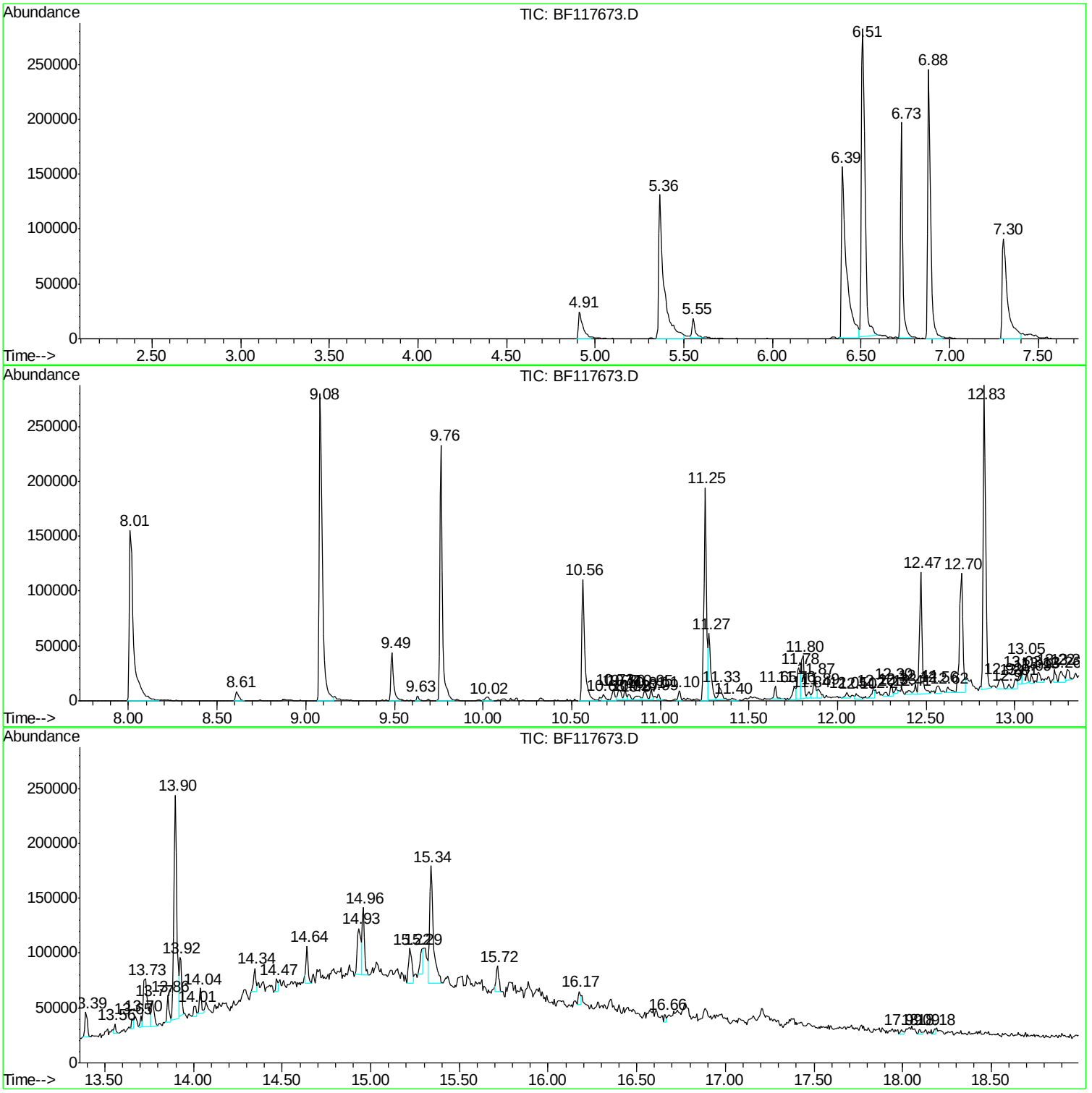
Instrument :
BNA_F
ClientSampleId :
18-12-(0-2.5)

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\BF103119\
Data File : BF117673.D
Acq On : 31 Oct 2019 22:01
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Sample : K5541-15 2X
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

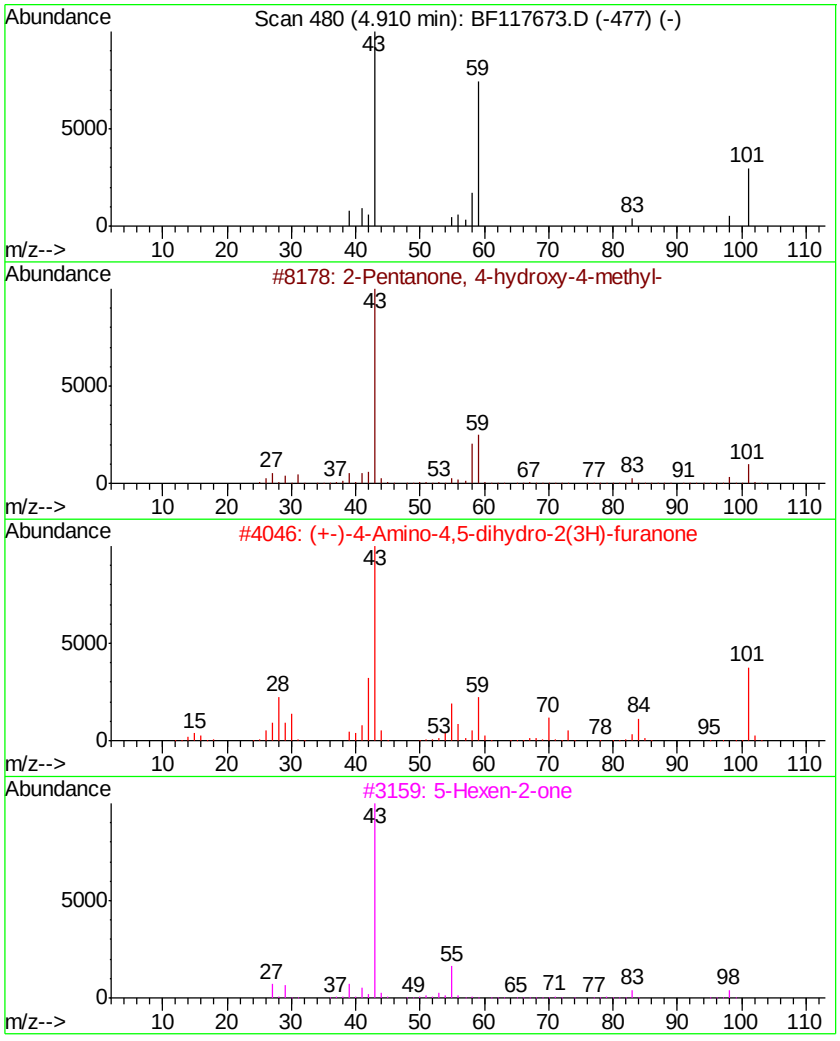
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

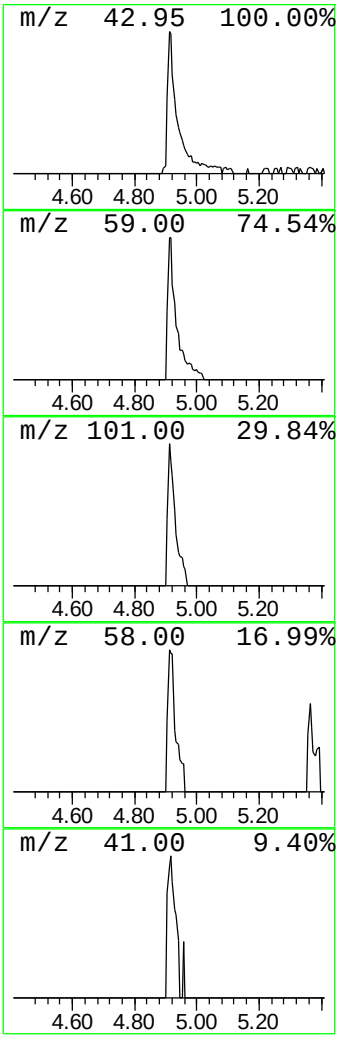
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.56 ng	42267	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Nonanone	142	C9H18O	000821-55-6	9





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

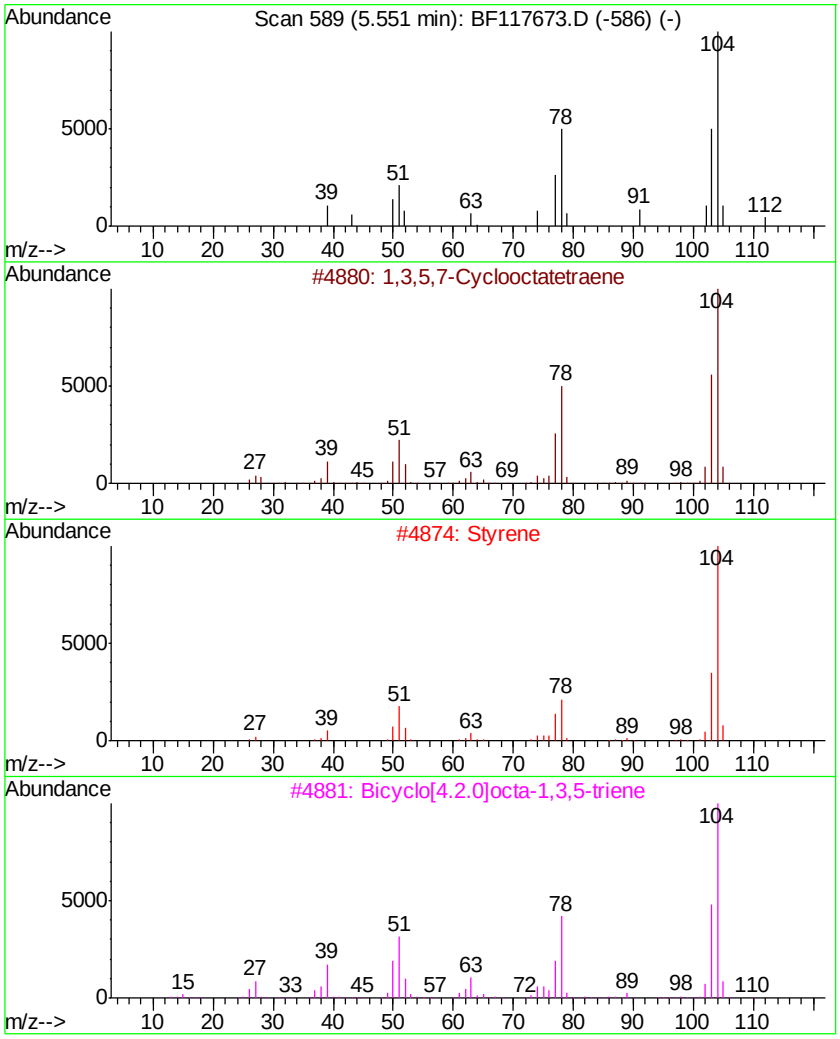
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

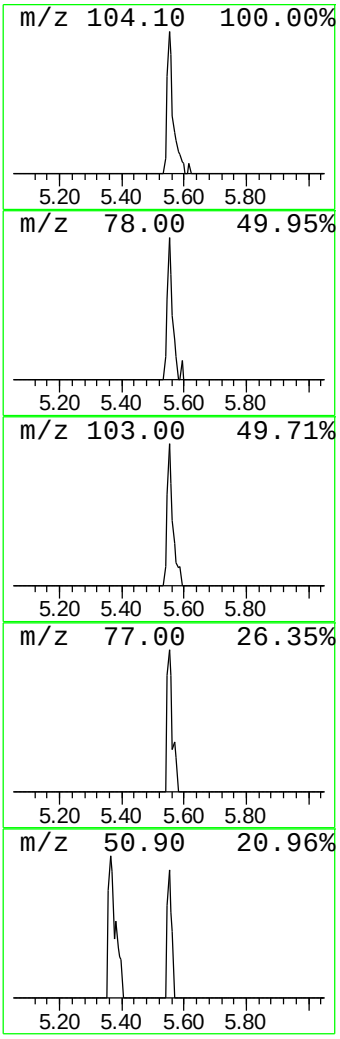
****

Peak Number 2 1,3,5,7-Cyclooctatetraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	2.49 ng	23048	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	91
2	Styrene	104	C8H8	000100-42-5	91
3	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	90
4	Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	64
5	3(2H)-Furanone, dihydro-2,2-dime...	190	C12H14O2	063678-00-2	53





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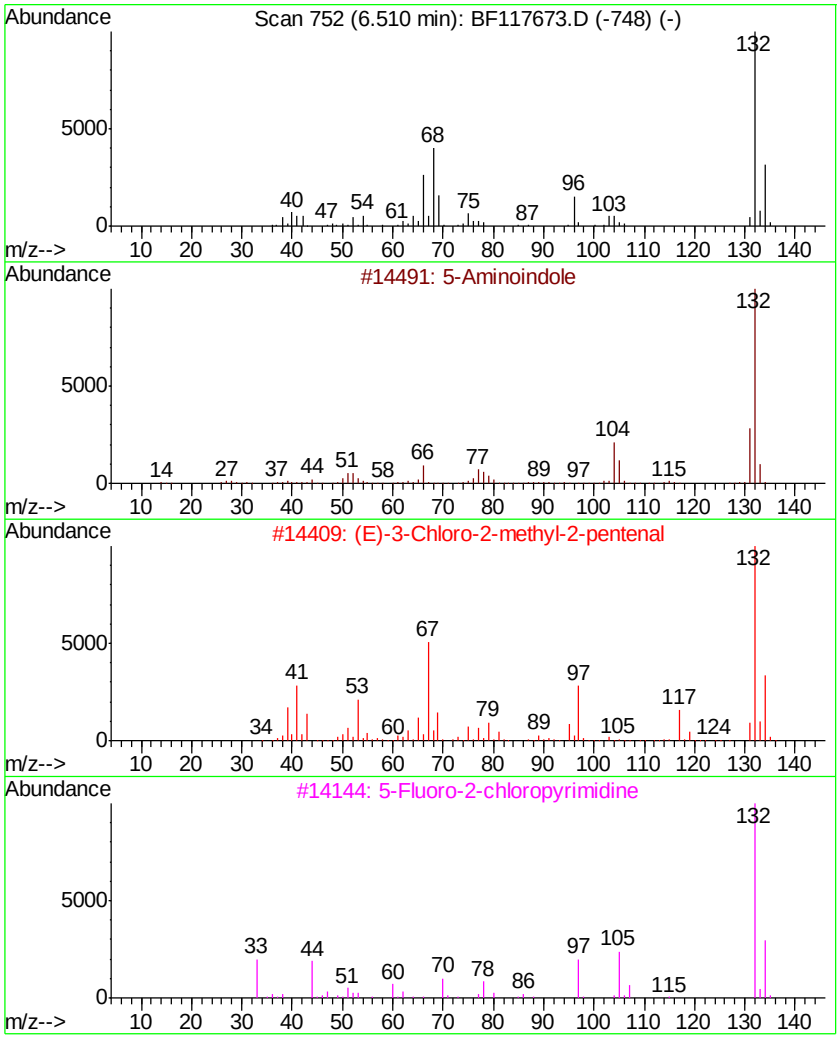
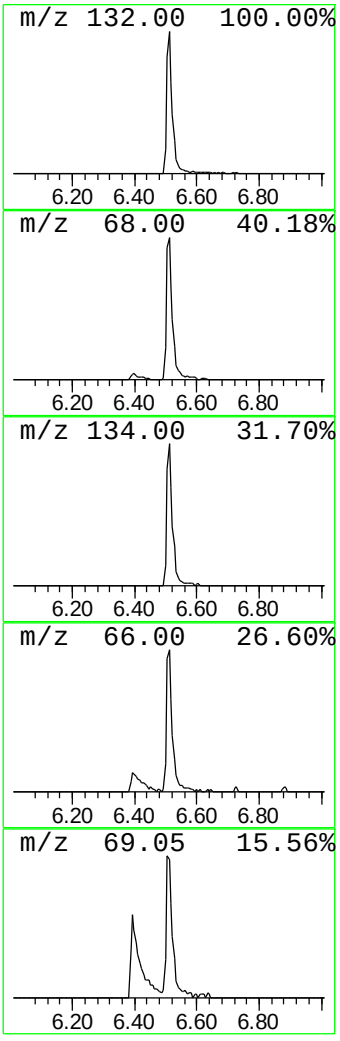
****

Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	40.14 ng	372092	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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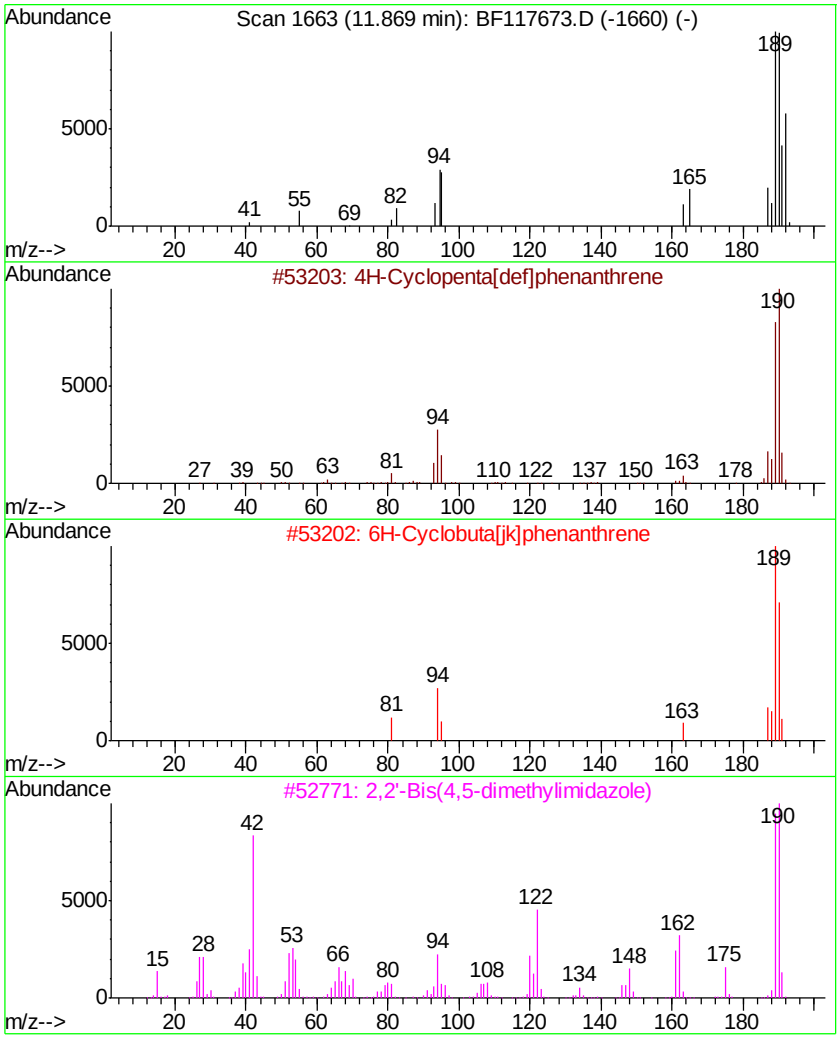
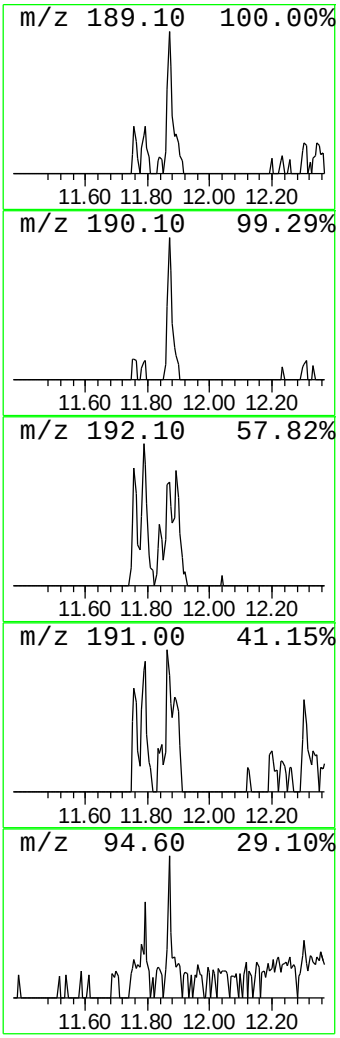
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.30 ng	22565	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	37
5	Methyl diselenide	190	C2H6Se2	007101-31-7	35





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Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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

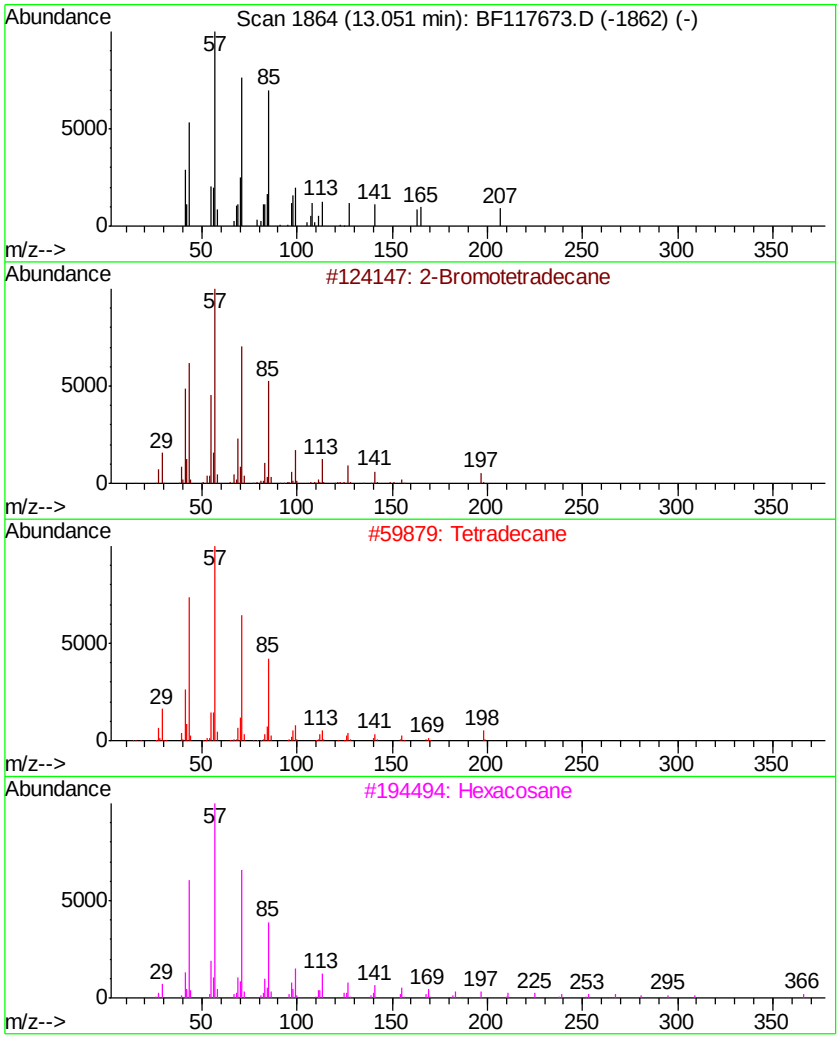
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

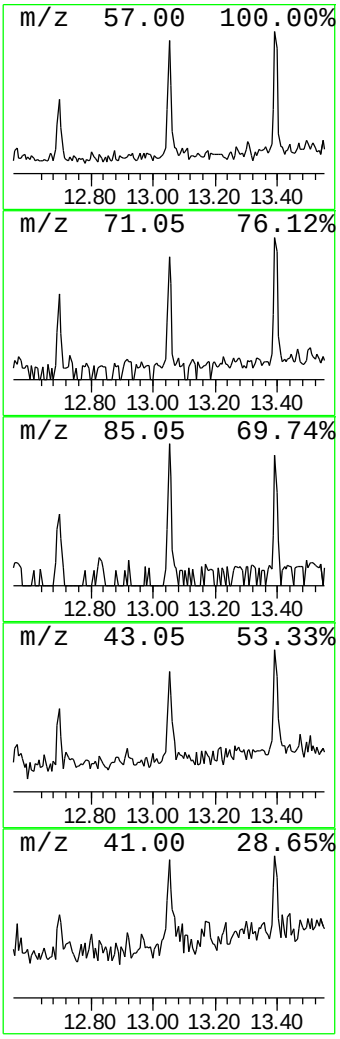
****

Peak Number 6 2-Bromotetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	2.14 ng	26916	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	64
2	Tetradecane	198	C14H30	000629-59-4	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Heneicosane	296	C21H44	000629-94-7	64
5	Pentacosane	352	C25H52	000629-99-2	64





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Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

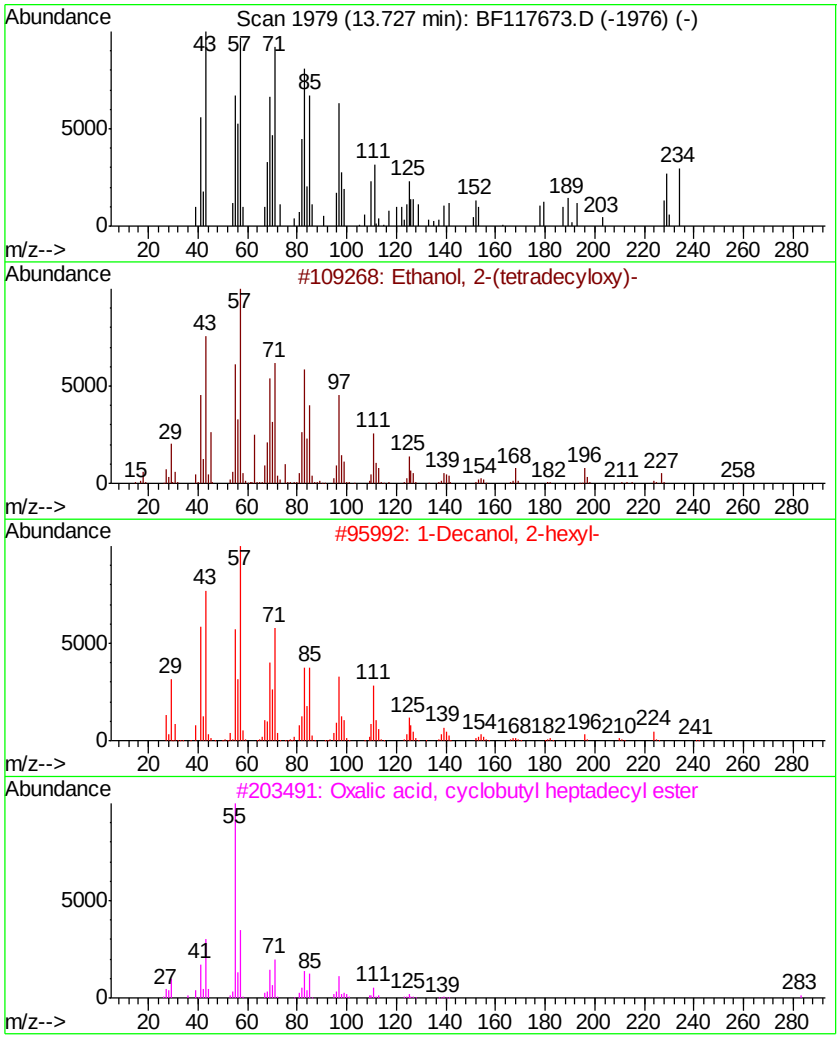
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

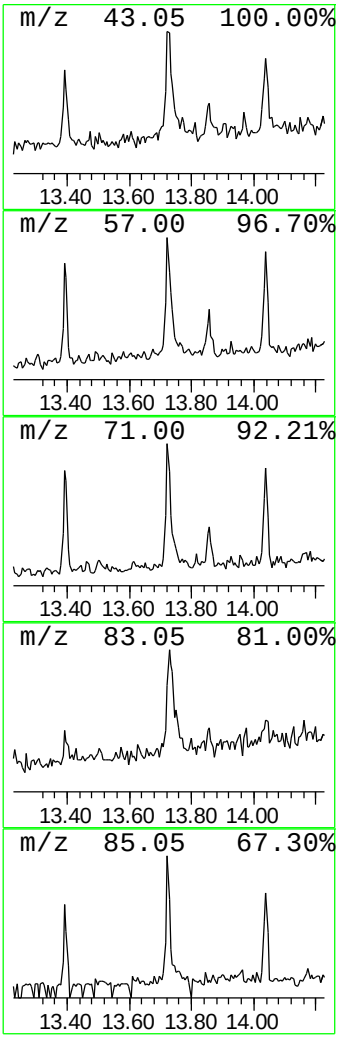
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.59 ng	70270	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64
3	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	59
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	52
5	1-Heptacosanol	396	C27H56O	002004-39-9	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117673.D
Acq On : 31 Oct 2019 22:01
Operator : JU
Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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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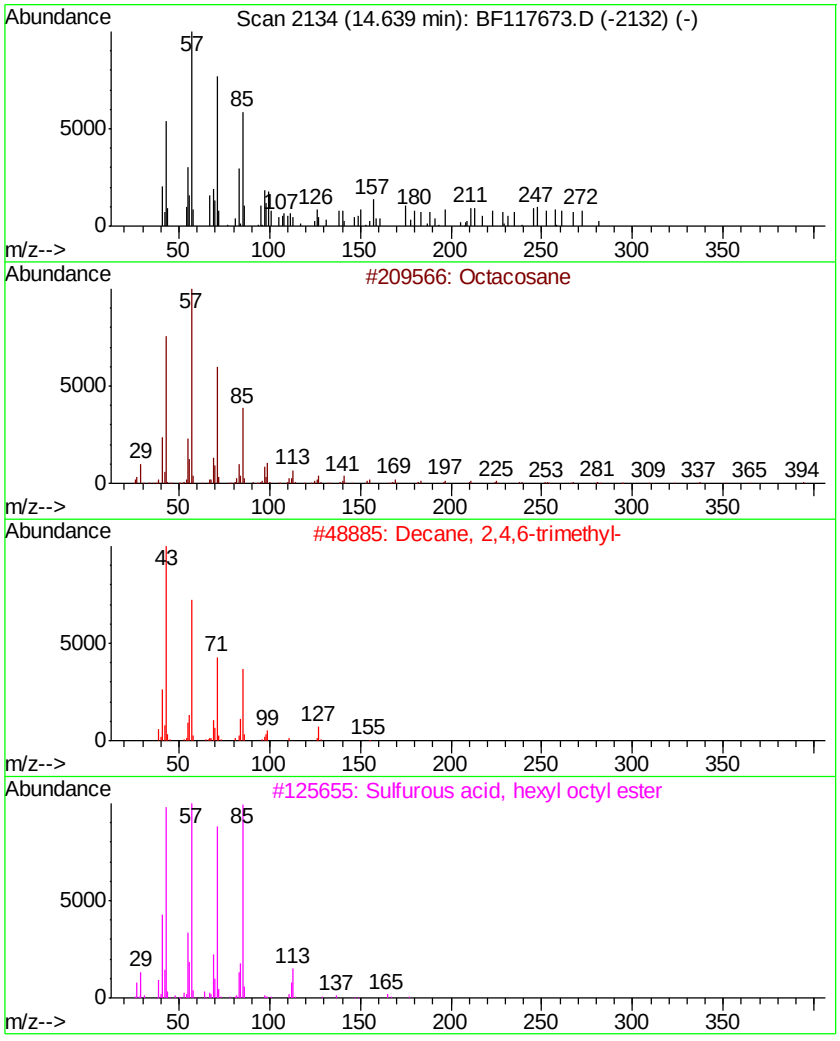
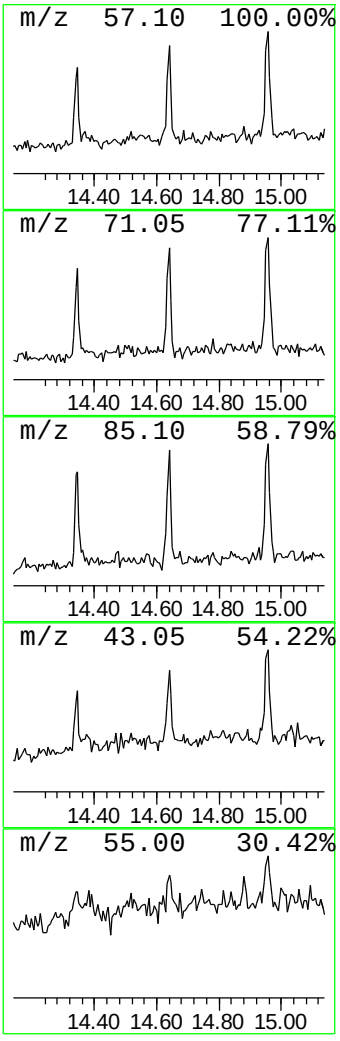
Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.53 ng	29786	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	53
2	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	52
3	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	50
4	Decane, 4-ethyl-	170	C12H26	001636-44-8	50
5	Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	50





Library Search Compound Report

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Data File : BF117673.D
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Operator : JU
Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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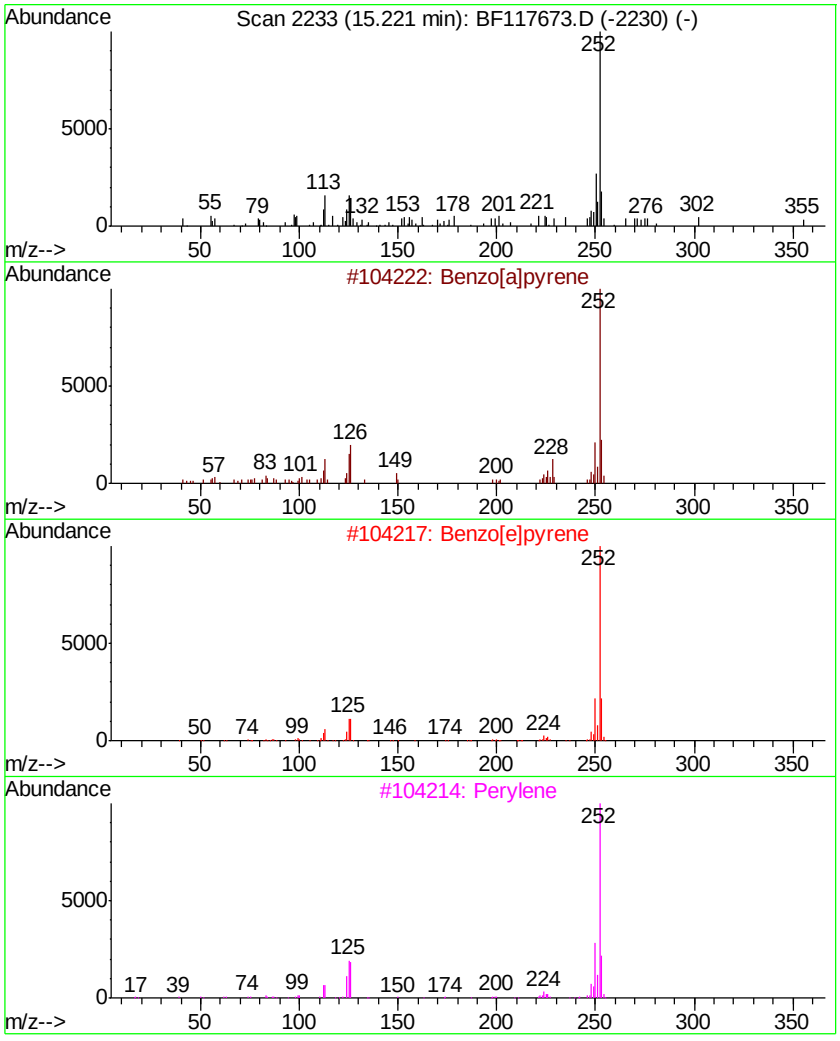
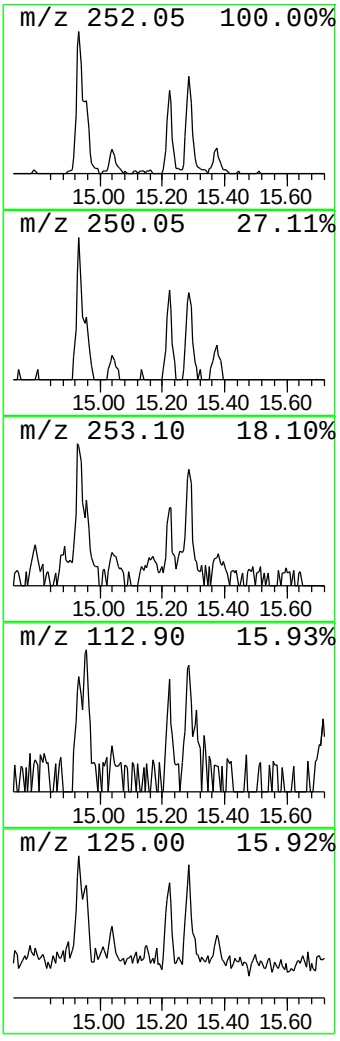
Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	4.38 ng	36972	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	83
2	Benzo[e]pyrene	252	C20H12	000192-97-2	64
3	Perylene	252	C20H12	000198-55-0	60
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	58
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117673.D
Acq On : 31 Oct 2019 22:01
Operator : JU
Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-12-(0-2.5)

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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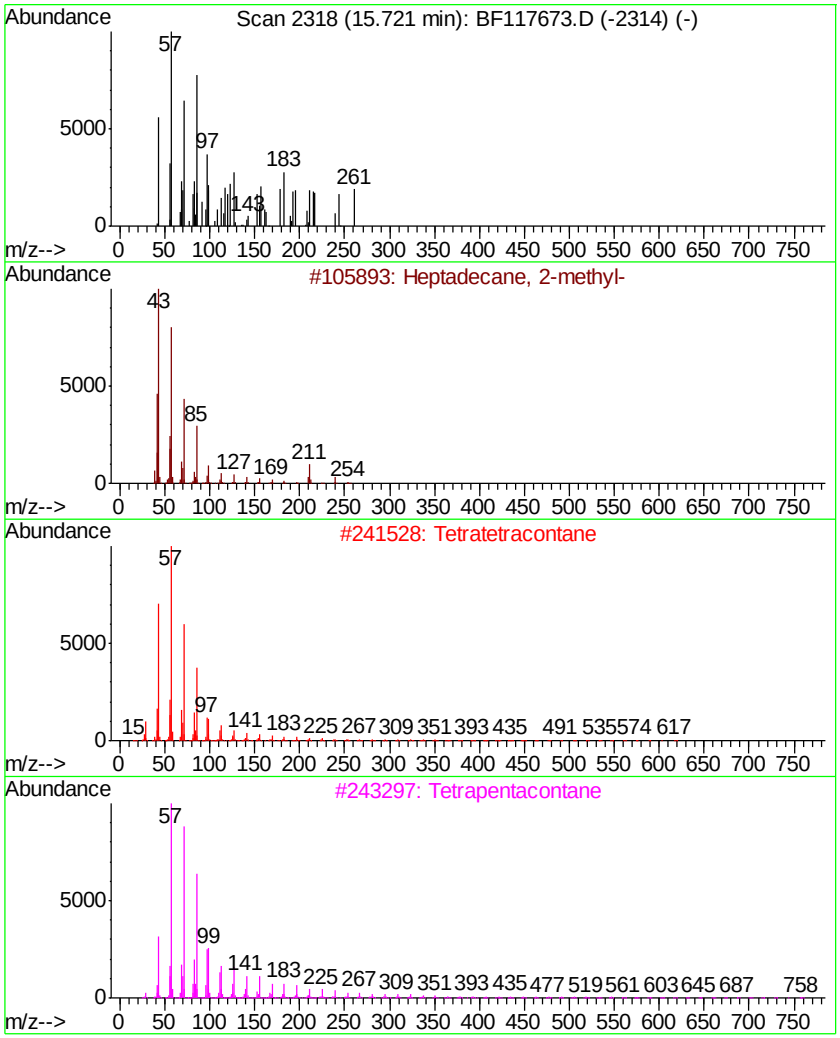
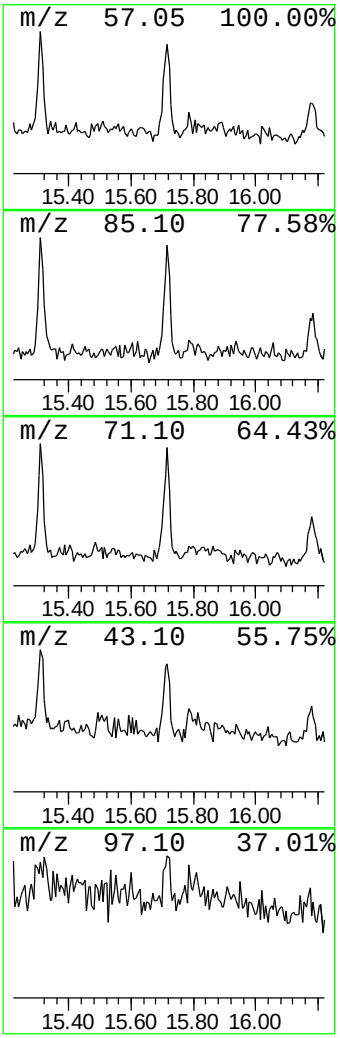
Peak Number 10 Heptadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.20 ng	26978	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	59
2	Tetratetracontane	619	C44H90	007098-22-8	59
3	Tetrapentacontane	759	C54H110	005856-66-6	59
4	Octacosane	394	C28H58	000630-02-4	59
5	2-methyltetracosane	352	C25H52	1000376-72-6	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
Data File : BF117673.D
Acq On : 31 Oct 2019 22:01
Operator : JU
Sample : K5541-15 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-12-(0-2.5)

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
2-Pentanone, 4-hy...	4.91	4.6	ng	42267	1	6.73	185420	20.0
1,3,5,7-Cycloocta...	5.55	2.5	ng	23048	1	6.73	185420	20.0
unknown6.51	6.51	40.1	ng	372092	1	6.73	185420	20.0
4H-Cyclopenta[def...	11.87	2.3	ng	22565	4	11.25	196159	20.0
2-Bromotetradecane	13.05	2.1	ng	26916	5	13.90	251321	20.0
Ethanol, 2-(tetra...	13.73	5.6	ng	70270	5	13.90	251321	20.0
Octacosane	14.64	3.5	ng	29786	6	15.34	168650	20.0
Benzo[e]pyrene	15.22	4.4	ng	36972	6	15.34	168650	20.0
Heptadecane, 2-me...	15.72	3.2	ng	26978	6	15.34	168650	20.0