LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117724.D
Acq On : 8 Nov 2019 00:02
Operator : JU
Sample : K5722-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6-A

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-BF110619.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	2.228	18	24	34	rVB	1238464	1579786	25.27%	2.277%
2	5.151	515	521	528	rVB	979550	1180611	18.88%	1.702%
3	5.545	583	588	591	rBV	5492309	5029142	80.43%	7.249%
4	6.545	753	758	763	rBV	5035360	5495900	87.90%	7.921%
5	6.698	780	784	787	rBV	6006913	5482342	87.68%	7.902%
6	6.934	820	824	827	rBV	2260527	1758087	28.12%	2.534%
7	7.092	847	851	854	rVB	4906373	4325992	69.19%	6.235%
8	7.492	912	919	922	rBV	3841783	3389686	54.21%	4.886%
9	8.222	1037	1043	1045	rBV	2496008	2326136	37.20%	3.353%
10	9.298	1221	1226	1229	rBV	7501349	6252451	100.00%	9.012%
11	9.686	1289	1292	1296	rVB	710231	539156	8.62%	0.777%
12	9.839	1315	1318	1322	rVB	90563	72691	1.16%	0.105%
13	9.980	1338	1342	1345	rVB	3151793	2602523	41.62%	3.751%
14	10.527	1429	1435	1437	rBV2	62978	72150	1.15%	0.104%
15	10.598	1441	1447	1449	rBV3	68274	87764	1.40%	0.126%
16	10.680	1457	1461	1468	rVB5	49145	79516	1.27%	0.115%
17	10.769	1471	1476	1479	rVV	4463833	3829812	61.25%	5.520%
18	10.804	1479	1482	1488	rVB2	73490	97067	1.55%	0.140%
19	10.892	1494	1497	1502	rVB3	111610	155612	2.49%	0.224%
20	11.074	1524	1528	1531	rVB3	71895	94732	1.52%	0.137%
21	11.110	1531	1534	1540	rBV2	100699	139773	2.24%	0.201%
22	11.227	1545	1554	1559	rBV7	56308	145157	2.32%	0.209%
23	11.333	1565	1572	1575	rBV5	87176	142713	2.28%	0.206%
24	11.369	1575	1578	1582	rVB	80666	82860	1.33%	0.119%
25	11.469	1592	1595	1598	rBV	2813693	2589743	41.42%	3.733%
26	11.492	1598	1599	1603	rVV	835101	601872	9.63%	0.867%
27	11.539	1603	1607	1610	rVV2	170799	203349	3.25%	0.293%
28	11.580	1610	1614	1617	rVV2	78988	103308	1.65%	0.149%
29	11.692	1630	1633	1636	rBV2	70452	75493	1.21%	0.109%
30	11.874	1659	1664	1669	rVB3	73469	111828	1.79%	0.161%
31	11.974	1678	1681	1682	rBV	337643	269580	4.31%	0.389%
32	11.998	1682	1685	1689	rVB2	883044	907891	14.52%	1.309%
33	12.086	1697	1700	1702	rBV2	215424	222341	3.56%	0.320%
34	12.110	1702	1704	1708	rVB	205792	166031	2.66%	0.239%

LSC Area Percent Report

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Integrator: RTE
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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-BF110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.174	1710	1715	1718	rBV4	85543	114912	1.84%	0.166%
36	12.292	1733	1735	1742	rVB3	112065	118345	1.89%	0.171%
37	12.421	1754	1757	1760	rBV	108312	90640	1.45%	0.131%
38	12.527	1771	1775	1777	rBV	166520	170637	2.73%	0.246%
39	12.563	1777	1781	1783	rVV	160090	164663	2.63%	0.237%
40	12.610	1786	1789	1795	rVB	188119	200309	3.20%	0.289%
41	12.686	1799	1802	1808	rBV	1181137	987369	15.79%	1.423%
42	12.780	1815	1818	1821	rBV	259597	222589	3.56%	0.321%
43	12.916	1836	1841	1843	rBV	1081980	1103316	17.65%	1.590%
44	12.974	1847	1851	1854	rVB3	63278	94193	1.51%	0.136%
45	13.063	1862	1866	1869	rBV	5978136	5279154	84.43%	7.609%
46	13.133	1875	1878	1882	rBV2	118032	169767	2.72%	0.245%
47	13.227	1890	1894	1895	rBV3	75425	96179	1.54%	0.139%
48	13.245	1895	1897	1900	rVB2	113031	96681	1.55%	0.139%
49	13.351	1912	1915	1918	rBV2	138809	113307	1.81%	0.163%
50	13.751	1980	1983	1988	rBV	170913	181693	2.91%	0.262%
51	13.868	1999	2003	2006	rBV2	102330	143180	2.29%	0.206%
52	13.898	2006	2008	2010	rBV	84975	71574	1.14%	0.103%
53	13.957	2015	2018	2024	rVV2	830747	752672	12.04%	1.085%
54	14.121	2040	2046	2048	rBV2	2336220	2658969	42.53%	3.832%
55	14.145	2048	2050	2055	rVB	586091	488855	7.82%	0.705%
56	14.539	2115	2117	2121	rVB2	127678	115367	1.85%	0.166%
57	14.592	2124	2126	2130	rVB2	158025	166017	2.66%	0.239%
58	14.757	2151	2154	2158	rVB2	154873	139568	2.23%	0.201%
59	14.910	2178	2180	2184	rBV2	84024	83458	1.33%	0.120%
60	14.992	2191	2194	2202	rVB	616144	637859	10.20%	0.919%
61	15.180	2222	2226	2229	rBV	525392	750910	12.01%	1.082%
62	15.268	2238	2241	2243	rBV2	108134	116754	1.87%	0.168%
63	15.498	2276	2280	2285	rVB	329897	389244	6.23%	0.561%
64	15.562	2287	2291	2295	rVB	320010	395143	6.32%	0.570%
65	15.633	2298	2303	2306	rBV	1798091	2207129	35.30%	3.181%
66	16.186	2393	2397	2407	rVB7	120098	279305	4.47%	0.403%
67	17.156	2557	2562	2570	rVB2	165154	330690	5.29%	0.477%
68	17.615	2636	2640	2648	rVB	126969	238215	3.81%	0.343%

Sum of corrected areas: 69381758

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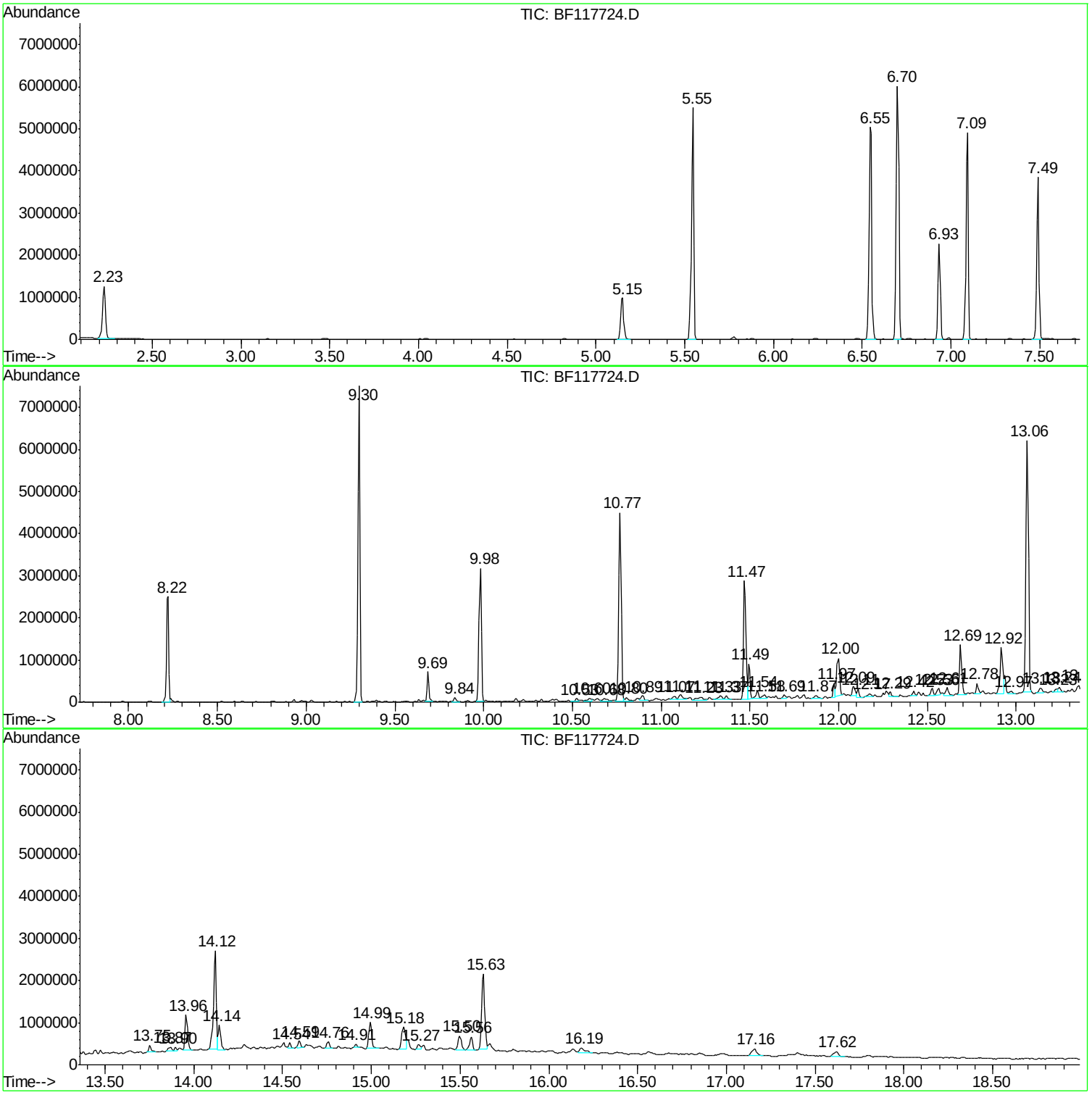
Instrument :
BNA_F
ClientSampleId :
6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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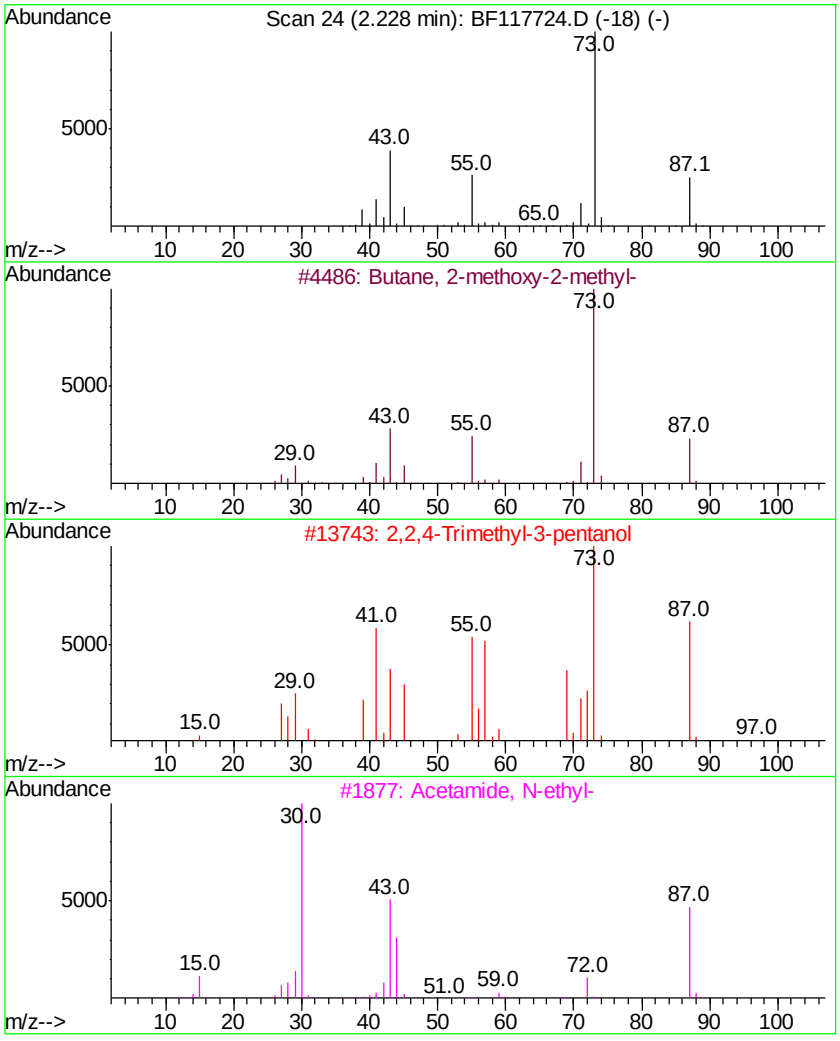
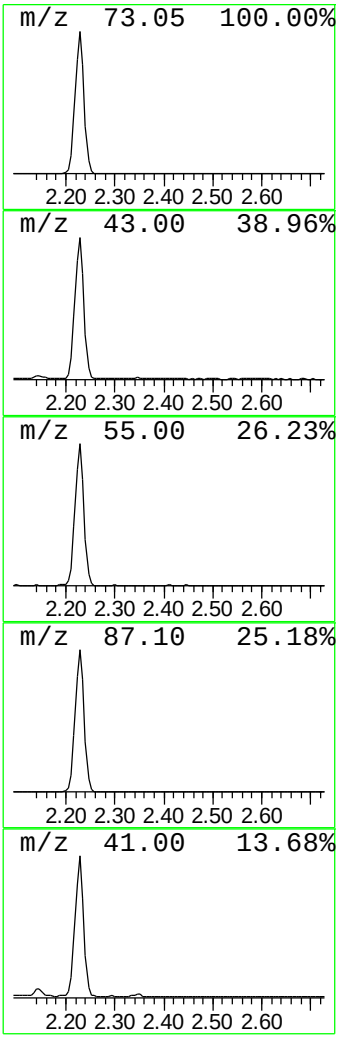
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	17.97 ng	1579790	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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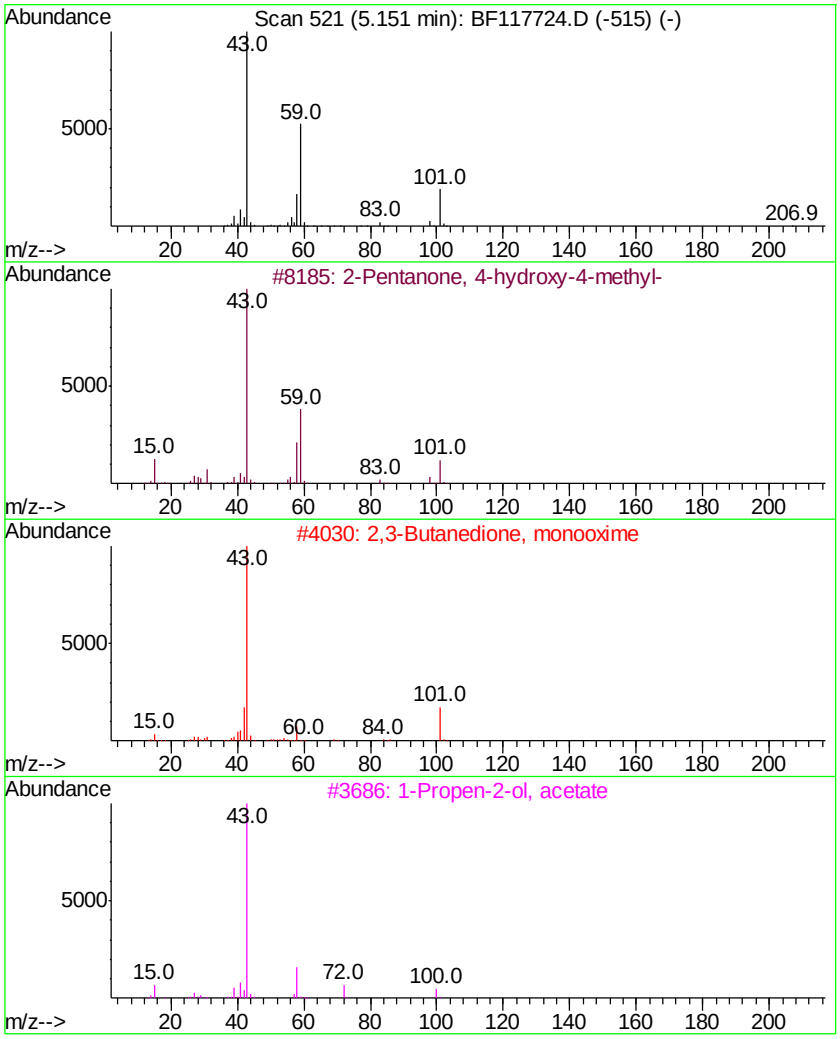
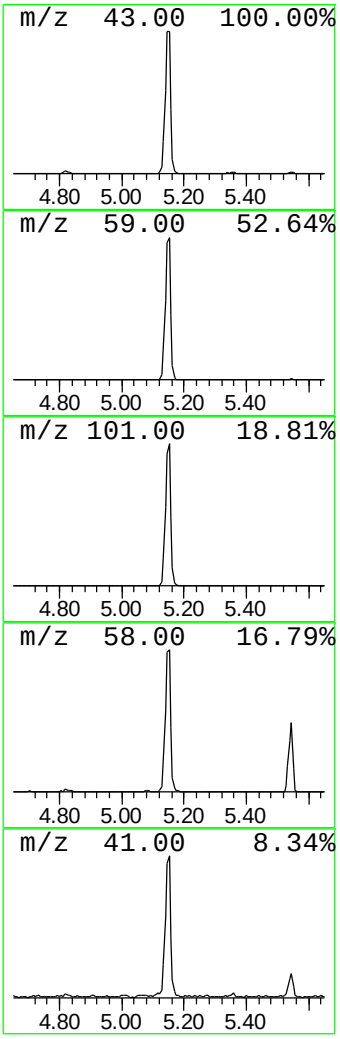
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.43 ng	1180610	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
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TIC Library : C:\DATABASE\NIST11.L
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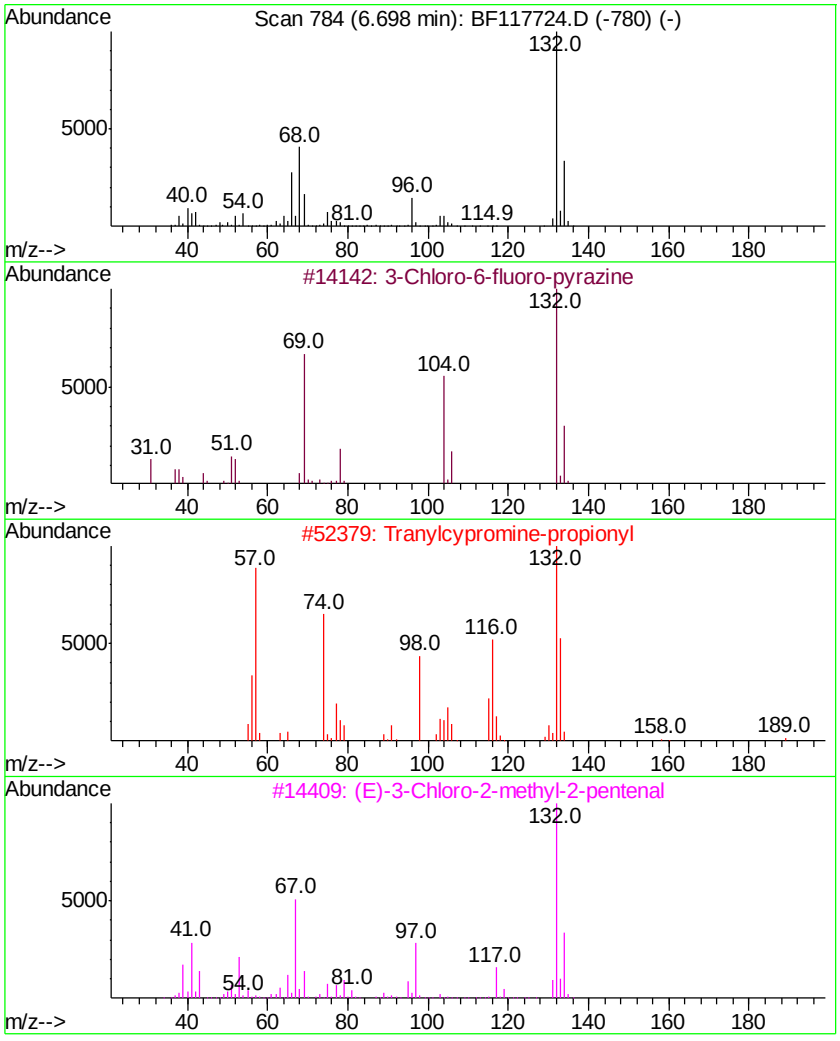
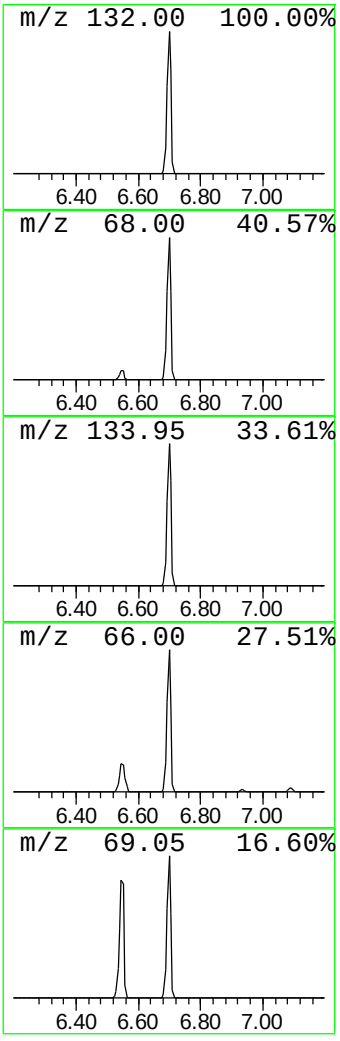
Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	62.37 ng	5482340	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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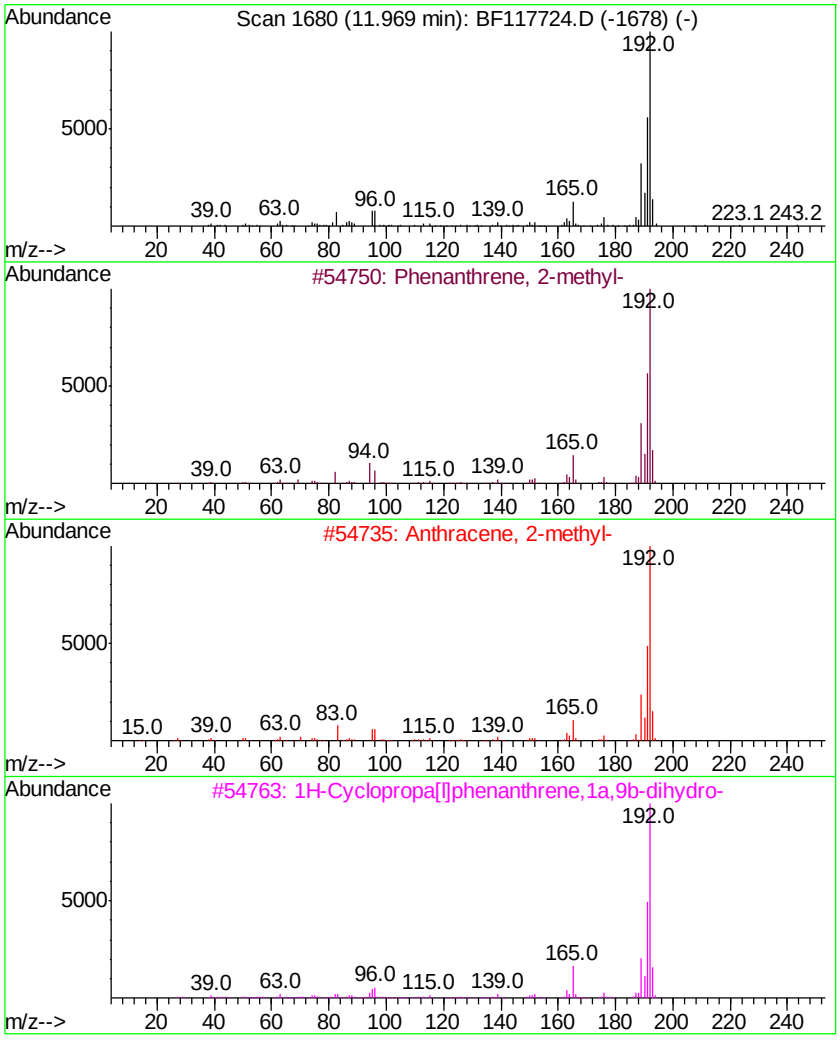
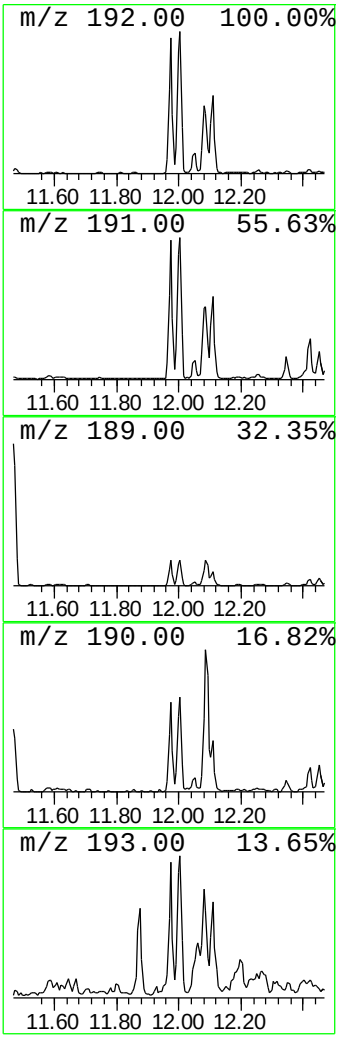
Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.08 ng	269580	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





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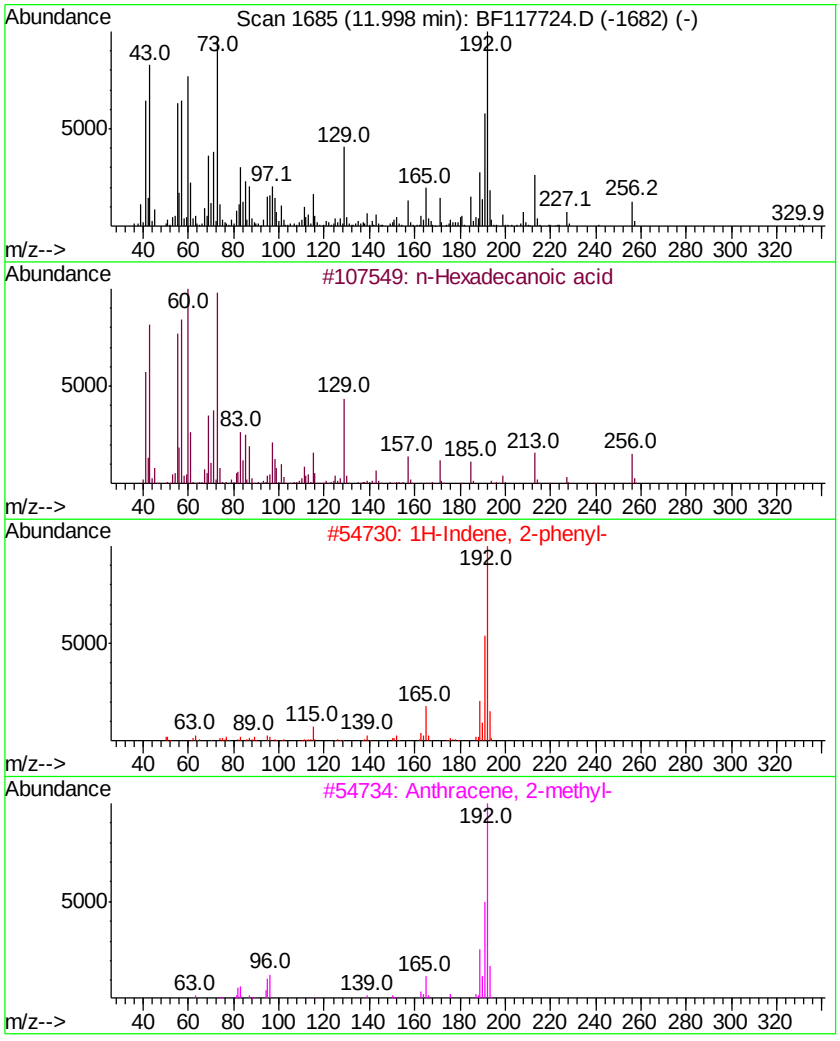
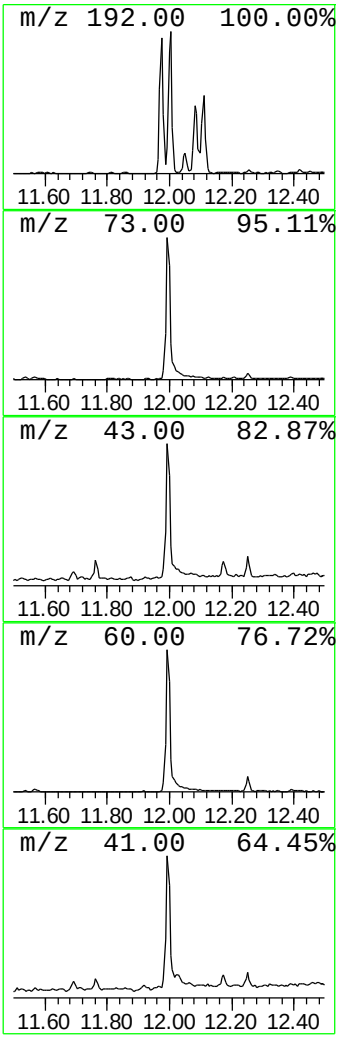
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	7.01 ng	907891	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	92
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
4	Octadecanoic acid	284	C18H36O2	000057-11-4	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	84





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

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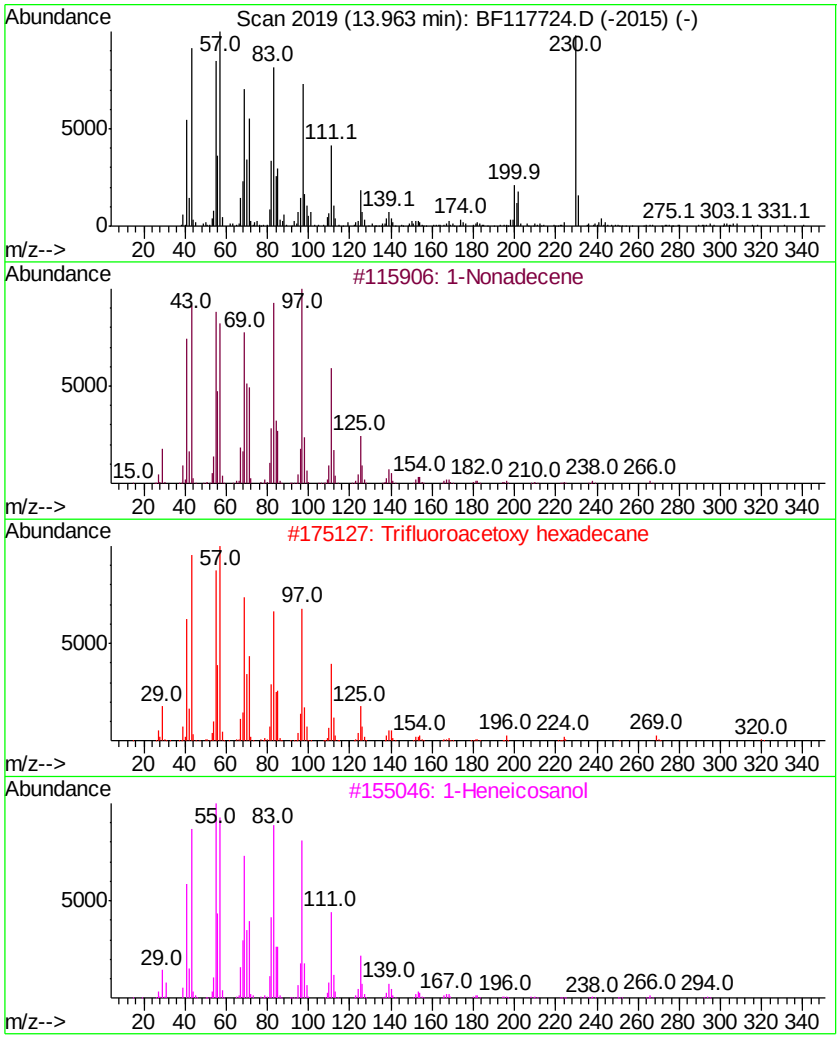
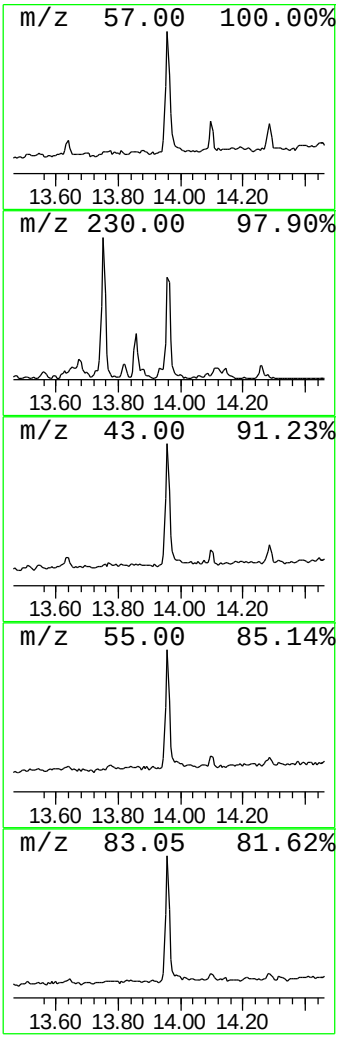
Peak Number 7 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.66 ng	752672	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	99
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
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Misc :
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Instrument : BNA_F
ClientSampleId : 6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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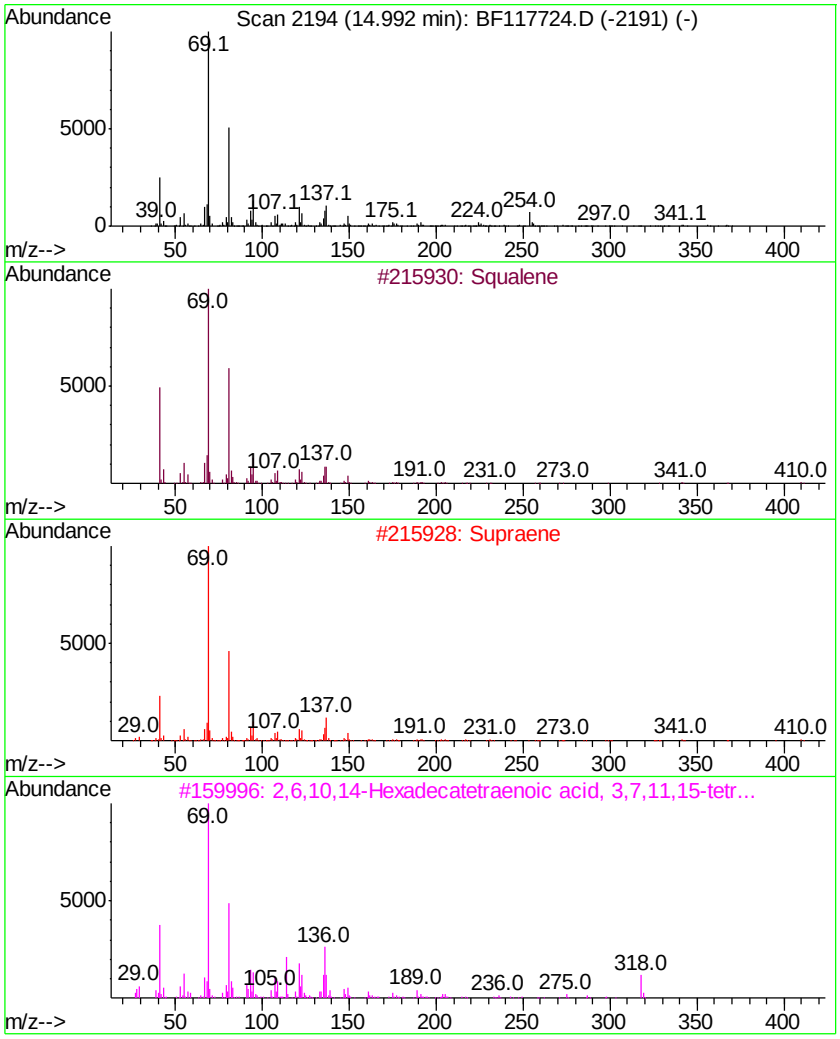
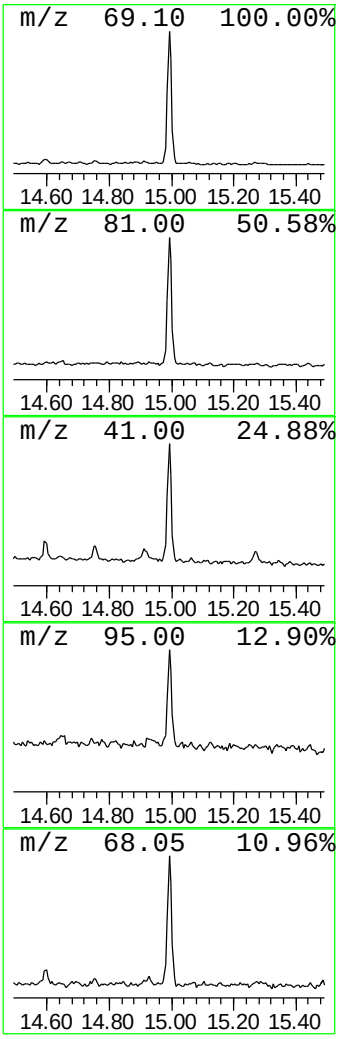
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	5.78 ng	637859	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64





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Acq On : 8 Nov 2019 00:02
Operator : JU
Sample : K5722-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6-A

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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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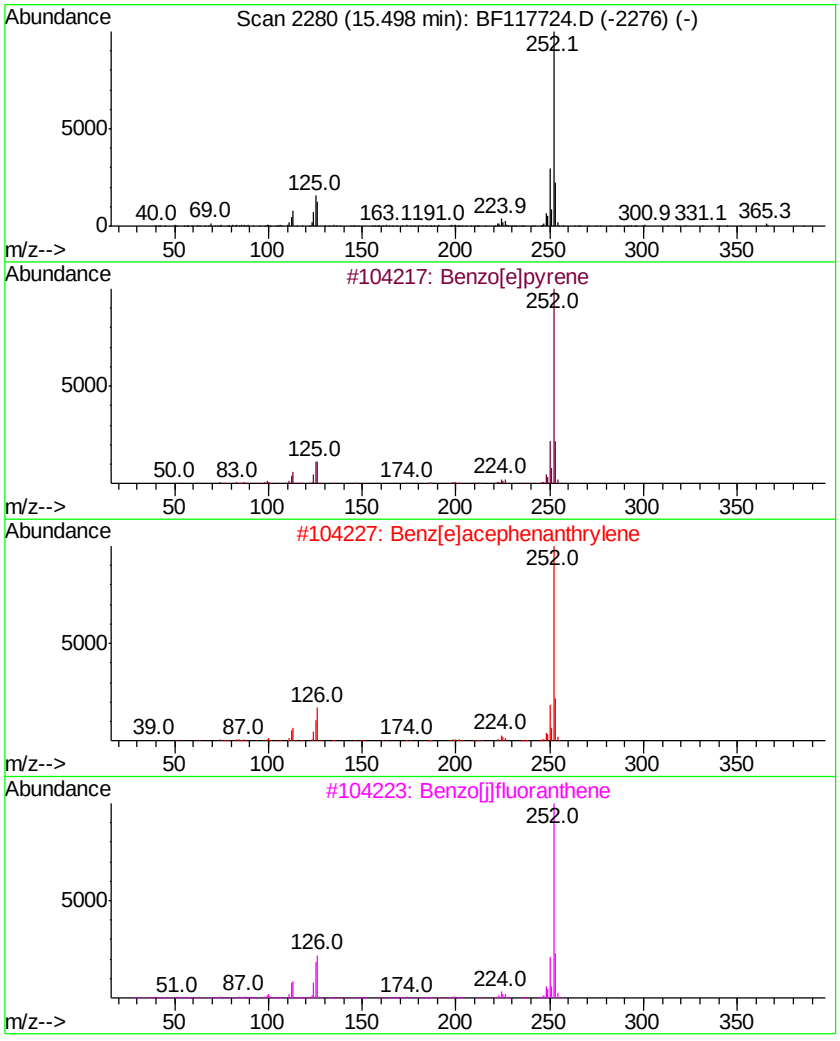
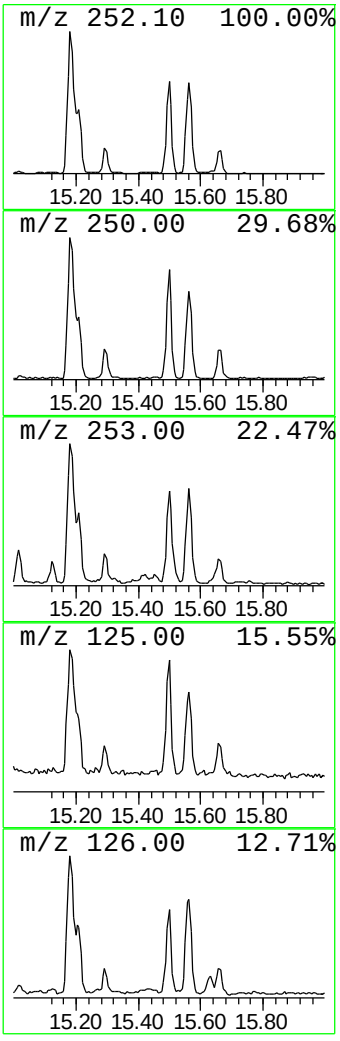
Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	3.53 ng	389244	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





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Data File : BF117724.D
Acq On : 8 Nov 2019 00:02
Operator : JU
Sample : K5722-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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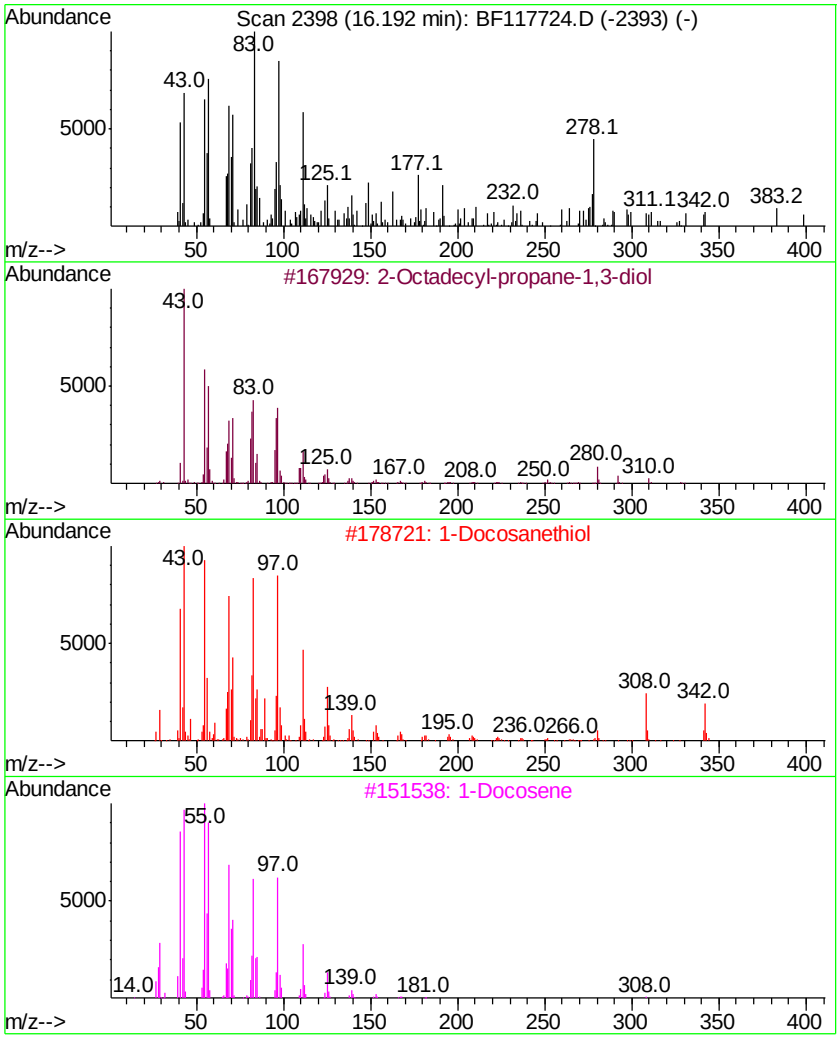
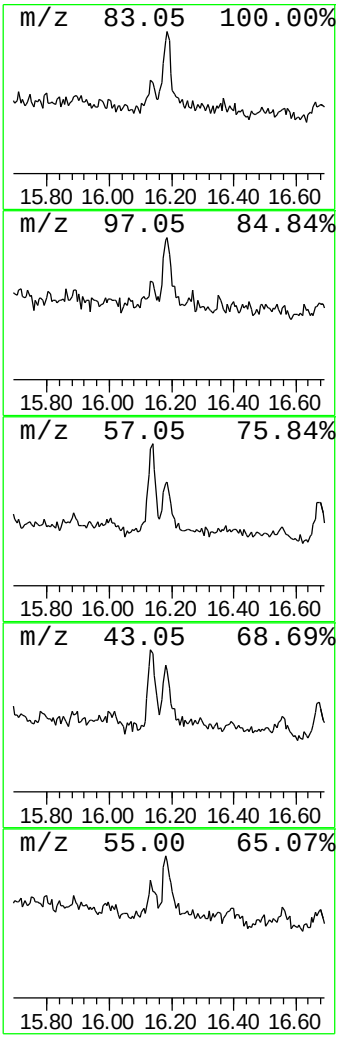
Peak Number 10 2-Octadecyl-propane-1,3-diol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.53 ng	279305	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	78
2	1-Docosanethiol	342	C22H46S	007773-83-3	68
3	1-Docosene	308	C22H44	001599-67-3	64
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	62
5	Octacosanol	410	C28H58O	000557-61-9	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110719\
Data File : BF117724.D
Acq On : 8 Nov 2019 00:02
Operator : JU
Sample : K5722-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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...	2.23	18.0	ng	1579790	1	6.93	1758090	20.0
2-Pentanone, 4-hy...	5.15	13.4	ng	1180610	1	6.93	1758090	20.0
unknown6.70	6.70	62.4	ng	5482340	1	6.93	1758090	20.0
Phenanthrene, 2-m...	11.97	2.1	ng	269580	4	11.47	2589740	20.0
n-Hexadecanoic acid	12.00	7.0	ng	907891	4	11.47	2589740	20.0
1-Nonadecene	13.96	5.7	ng	752672	5	14.12	2658970	20.0
Squalene	14.99	5.8	ng	637859	6	15.63	2207130	20.0
Benzo[e]pyrene	15.50	3.5	ng	389244	6	15.63	2207130	20.0
2-Octadecyl-propa...	16.19	2.5	ng	279305	6	15.63	2207130	20.0