LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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	19	24	39	rVB	1171958	1597647	25.04%	2.145%
2	3.451	229	232	245	rBV	48134	106415	1.67%	0.143%
3	5.145	515	520	527	rVB	1004990	1245864	19.53%	1.672%
4	5.545	583	588	591	rBV	5667618	5352755	83.89%	7.185%
5	6.551	753	759	763	rBV	5321127	5926812	92.89%	7.956%
6	6.698	780	784	788	rBV	6251076	5830578	91.38%	7.827%
7	6.933	820	824	827	rBV	2478216	1891786	29.65%	2.539%
8	6.986	830	833	838	rBV	117722	94906	1.49%	0.127%
9	7.092	847	851	854	rVB	5342393	4565435	71.55%	6.128%
10	7.492	914	919	922	rBV	4117921	3609439	56.57%	4.845%
11	8.222	1037	1043	1046	rBV	2760046	2549463	39.96%	3.422%
12	9.298	1221	1226	1229	rBV	7294107	6380784	100.00%	8.565%
13	9.686	1289	1292	1296	rVB	1156741	902931	14.15%	1.212%
14	9.839	1315	1318	1322	rVB	107130	86631	1.36%	0.116%
15	9.980	1338	1342	1345	rVB	3470753	2857592	44.78%	3.836%
16	10.769	1471	1476	1479	rBV	4886570	4195410	65.75%	5.632%
17	10.804	1479	1482	1488	rVB3	87444	100782	1.58%	0.135%
18	10.898	1494	1498	1505	rVB4	76587	121353	1.90%	0.163%
19	11.333	1565	1572	1576	rBV4	56228	89942	1.41%	0.121%
20	11.468	1591	1595	1598	rBV	3155280	2976920	46.65%	3.996%
21	11.492	1598	1599	1602	rVV	482385	304497	4.77%	0.409%
22	11.545	1602	1608	1611	rVV	325947	322083	5.05%	0.432%
23	11.692	1628	1633	1636	rBV	142383	145376	2.28%	0.195%
24	11.974	1675	1681	1682	rBV	166903	159770	2.50%	0.214%
25	11.992	1682	1684	1688	rVB2	568001	591063	9.26%	0.793%
26	12.080	1696	1699	1702	rBV2	155975	184013	2.88%	0.247%
27	12.104	1702	1703	1708	rVB	121771	99745	1.56%	0.134%
28	12.174	1708	1715	1718	rBV3	86079	117491	1.84%	0.158%
29	12.286	1733	1734	1742	rVB2	109286	89304	1.40%	0.120%
30	12.521	1771	1774	1777	rBV2	124654	125624	1.97%	0.169%
31	12.563	1777	1781	1783	rVV	121111	132599	2.08%	0.178%
32	12.604	1786	1788	1794	rVB2	98325	118283	1.85%	0.159%
33	12.686	1799	1802	1805	rBV	1124571	907958	14.23%	1.219%
34	12.721	1805	1808	1811	rVB2	218536	178037	2.79%	0.239%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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

35	12.780	1815	1818	1821	rBV	227326	199424	3.13%	0.268%
36	12.845	1826	1829	1832	rVV4	97382	135260	2.12%	0.182%
37	12.915	1835	1841	1844	rVV	1145065	1150164	18.03%	1.544%
38	12.962	1847	1849	1854	rVB2	59144	83006	1.30%	0.111%
39	13.062	1862	1866	1869	rBV	6717582	5826825	91.32%	7.822%
40	13.133	1874	1878	1881	rBV2	111043	153754	2.41%	0.206%
41	13.221	1890	1893	1895	rBV2	88102	113154	1.77%	0.152%
42	13.245	1895	1897	1900	rVB	108761	90113	1.41%	0.121%
43	13.351	1911	1915	1917	rBV2	152695	159952	2.51%	0.215%
44	13.445	1928	1931	1933	rVB	93853	83907	1.31%	0.113%
45	13.474	1933	1936	1939	rBV2	94017	89014	1.40%	0.119%
46	13.751	1980	1983	1988	rVB	166770	153126	2.40%	0.206%
47	13.862	1997	2002	2005	rBV2	113299	182015	2.85%	0.244%
48	13.957	2015	2018	2024	rVB2	702060	654520	10.26%	0.879%
49	14.115	2037	2045	2048	rBV2	2569769	3047939	47.77%	4.091%
50	14.145	2048	2050	2056	rVB	618543	563185	8.83%	0.756%
51	14.286	2070	2074	2079	rVB5	111522	173047	2.71%	0.232%
52	14.504	2108	2111	2114	rVB	123997	117163	1.84%	0.157%
53	14.539	2114	2117	2120	rVB	127235	118954	1.86%	0.160%
54	14.592	2121	2126	2130	rBV3	212451	241364	3.78%	0.324%
55	14.909	2176	2180	2183	rBV2	171093	191794	3.01%	0.257%
56	14.992	2190	2194	2201	rBV	348364	408450	6.40%	0.548%
57	15.180	2220	2226	2229	rBV	574511	935738	14.66%	1.256%
58	15.268	2237	2241	2243	rBV2	157831	208649	3.27%	0.280%
59	15.292	2243	2245	2249	rVB	116180	110831	1.74%	0.149%
60	15.386	2258	2261	2267	rBV5	41183	82004	1.29%	0.110%
61	15.492	2275	2279	2285	rVB	342571	463790	7.27%	0.623%
62	15.556	2286	2290	2296	rVV	345719	406246	6.37%	0.545%
63	15.627	2296	2302	2306	rVV	1973330	2448311	38.37%	3.286%
64	15.668	2306	2309	2315	rVB4	196620	316178	4.96%	0.424%
65	16.133	2383	2388	2392	rBV	139501	229834	3.60%	0.309%
66	16.556	2456	2460	2474	rVB8	65878	164193	2.57%	0.220%
67	16.668	2474	2479	2489	rBV6	81387	234422	3.67%	0.315%
68	16.974	2527	2531	2537	rVB5	50261	111970	1.75%	0.150%
69	17.150	2555	2561	2569	rBV2	177125	355616	5.57%	0.477%
70	17.303	2583	2587	2592	rBV3	43433	101488	1.59%	0.136%
71	17.397	2599	2603	2618	rVB5	60587	166590	2.61%	0.224%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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

72	17.609	2634	2639	2646	rVB	133332	264956	4.15%	0.356%

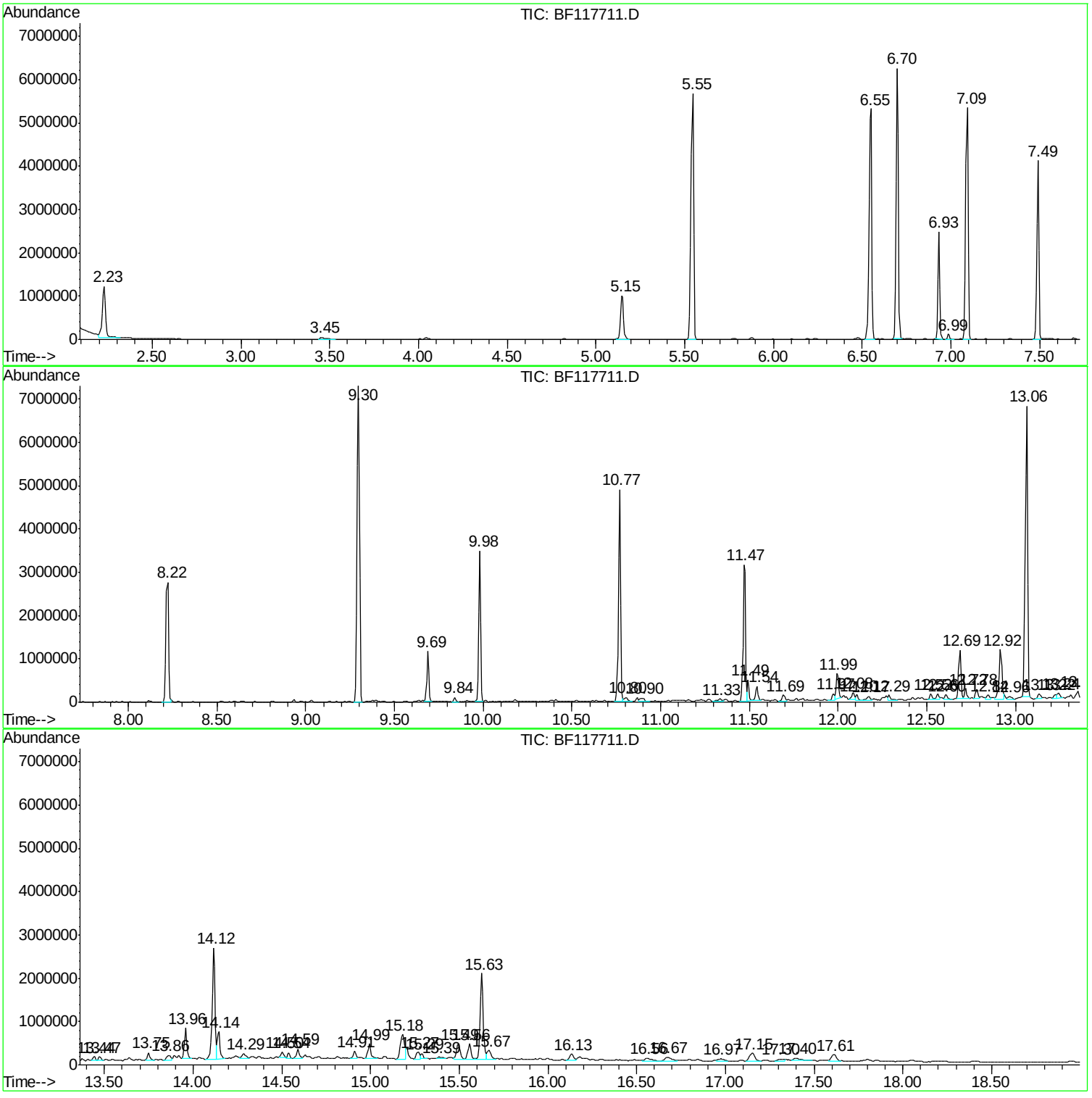
Sum of corrected areas: 74496234

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
8-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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

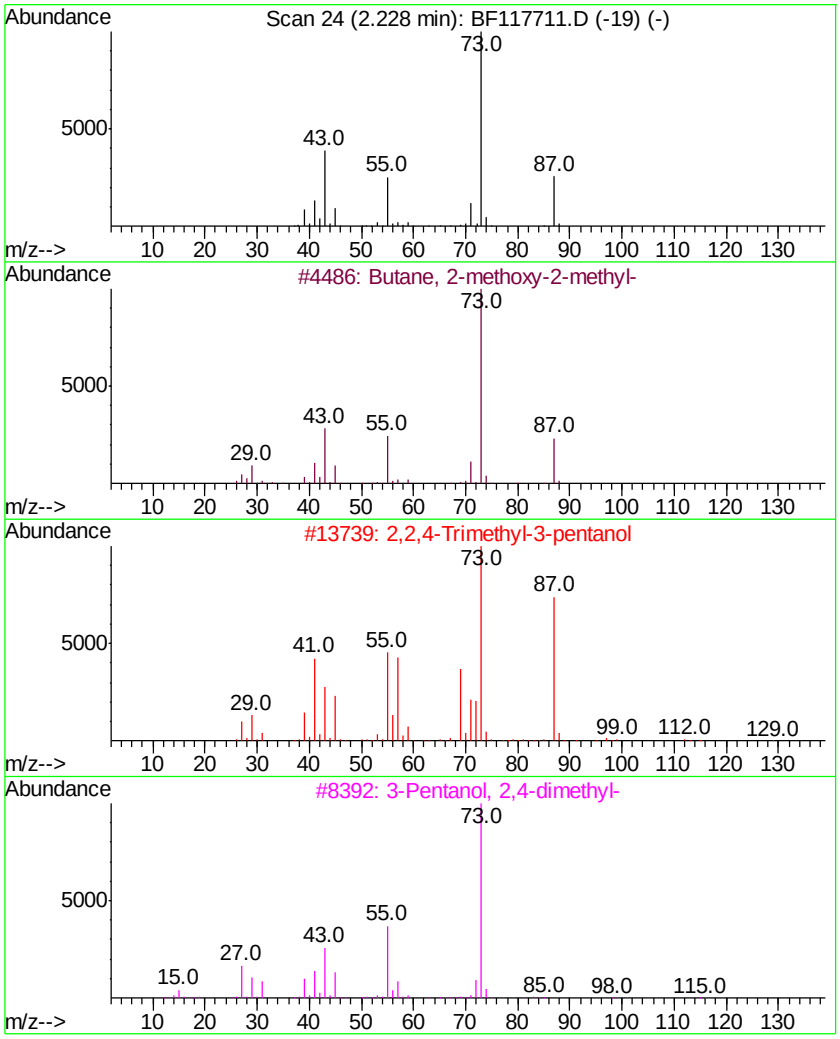
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

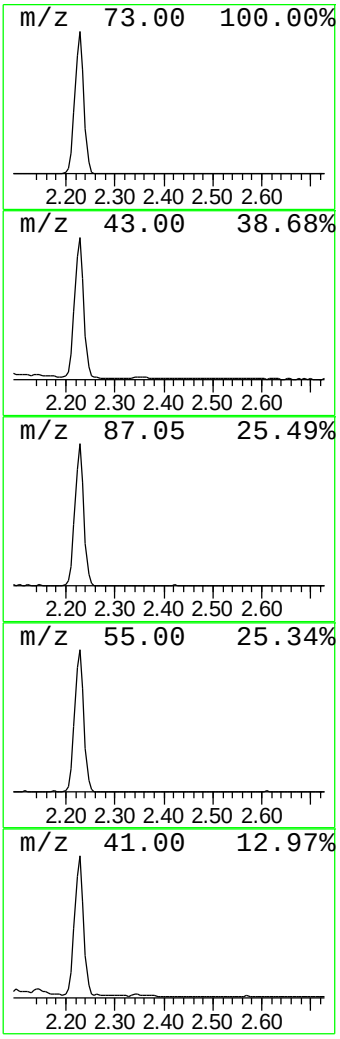
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	16.89 ng	1597650	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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

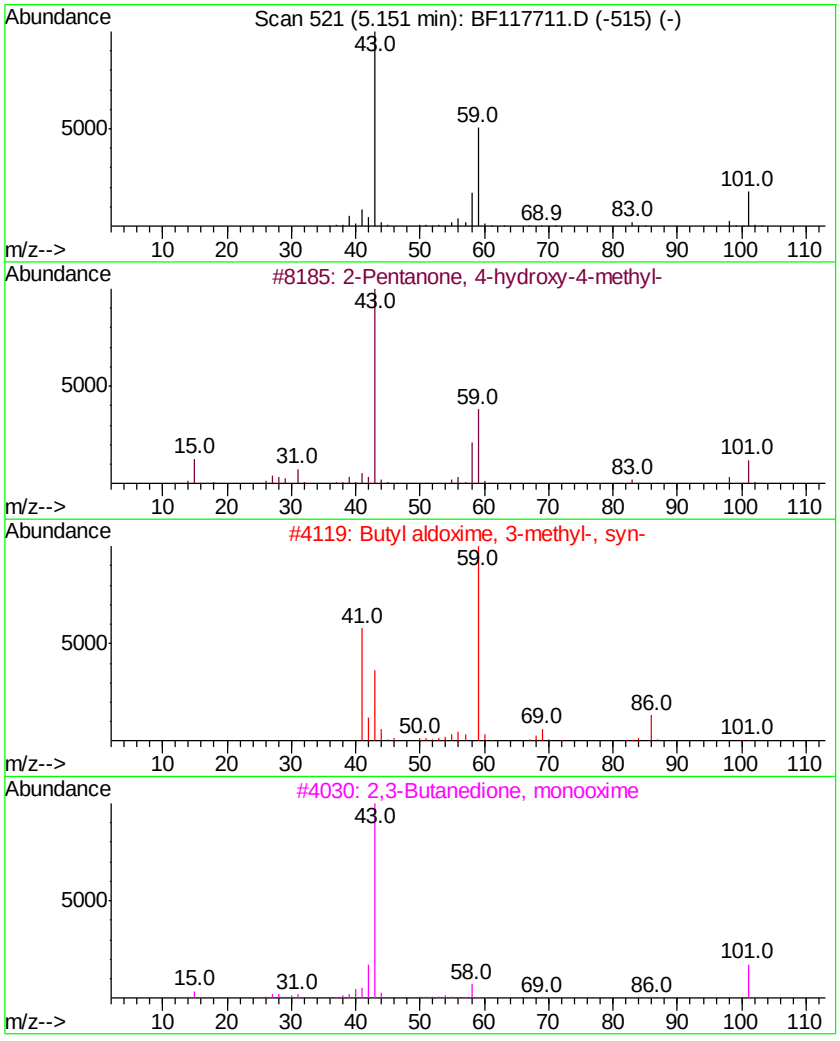
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

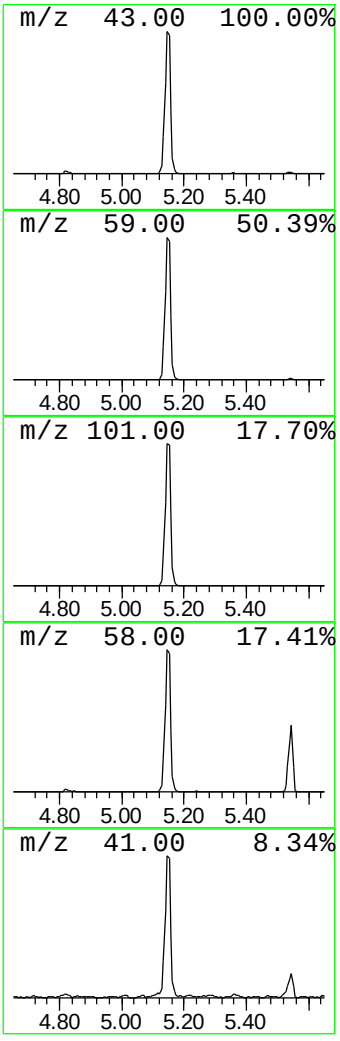
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.17 ng	1245860	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	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

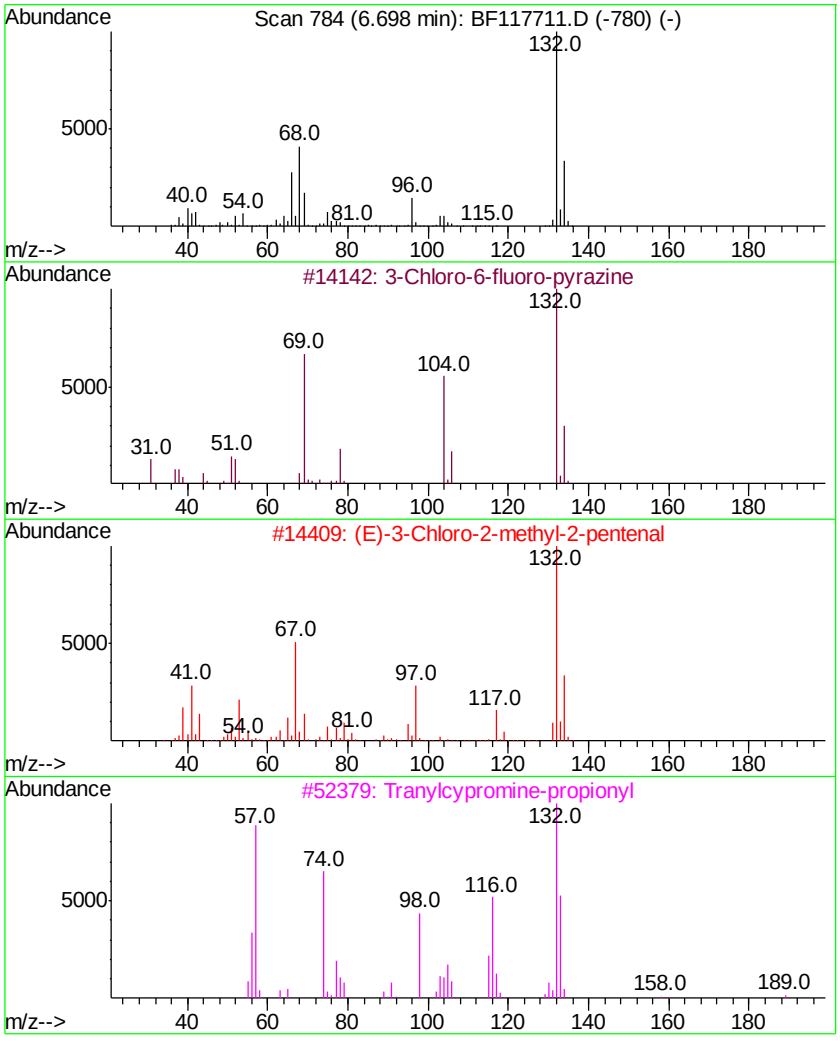
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

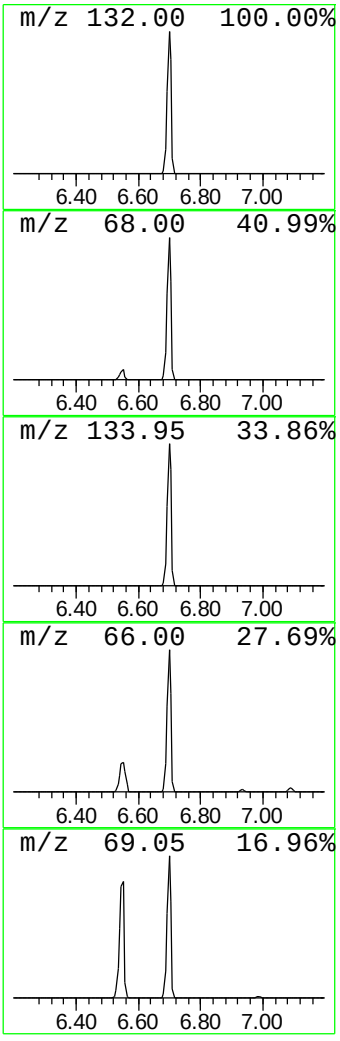
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	61.64 ng	5830580	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

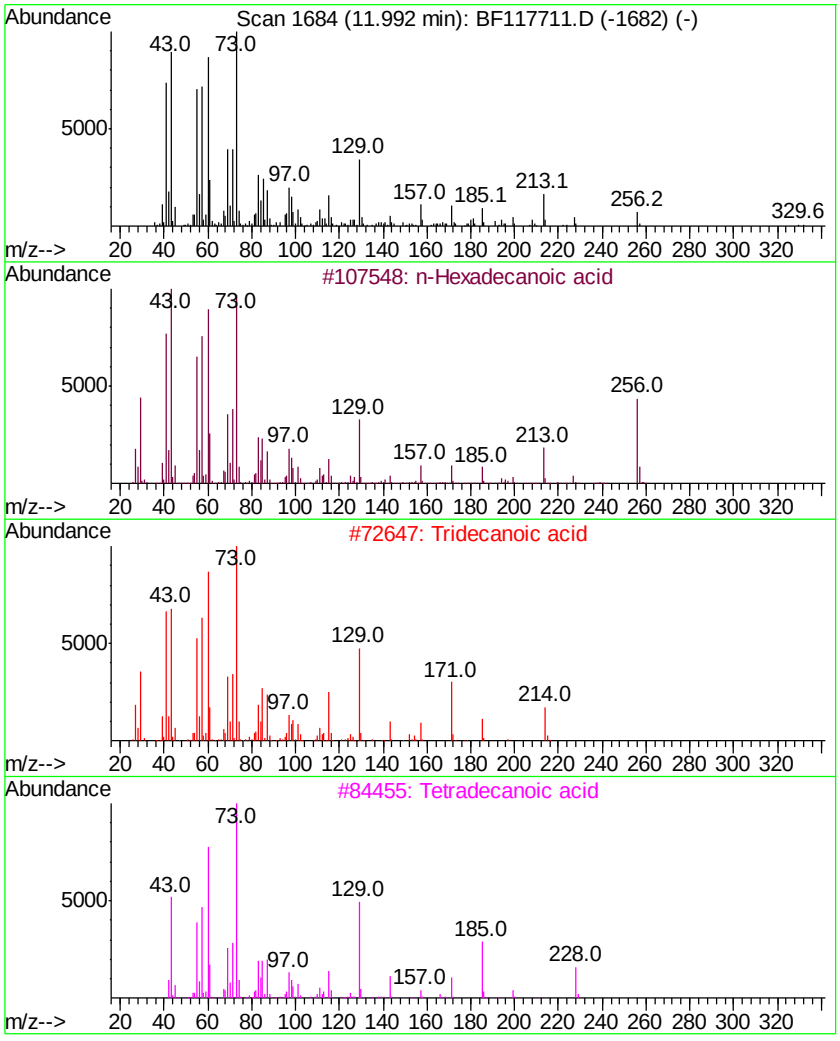
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

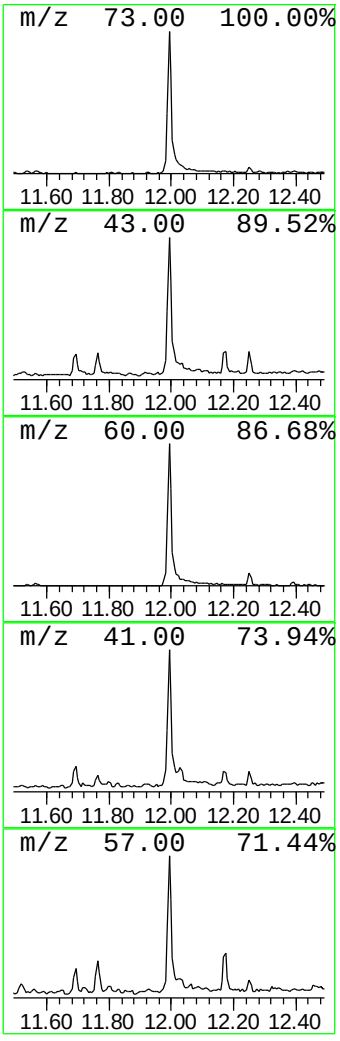
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.97 ng	591063	Phenanthrene-d10	11.47

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

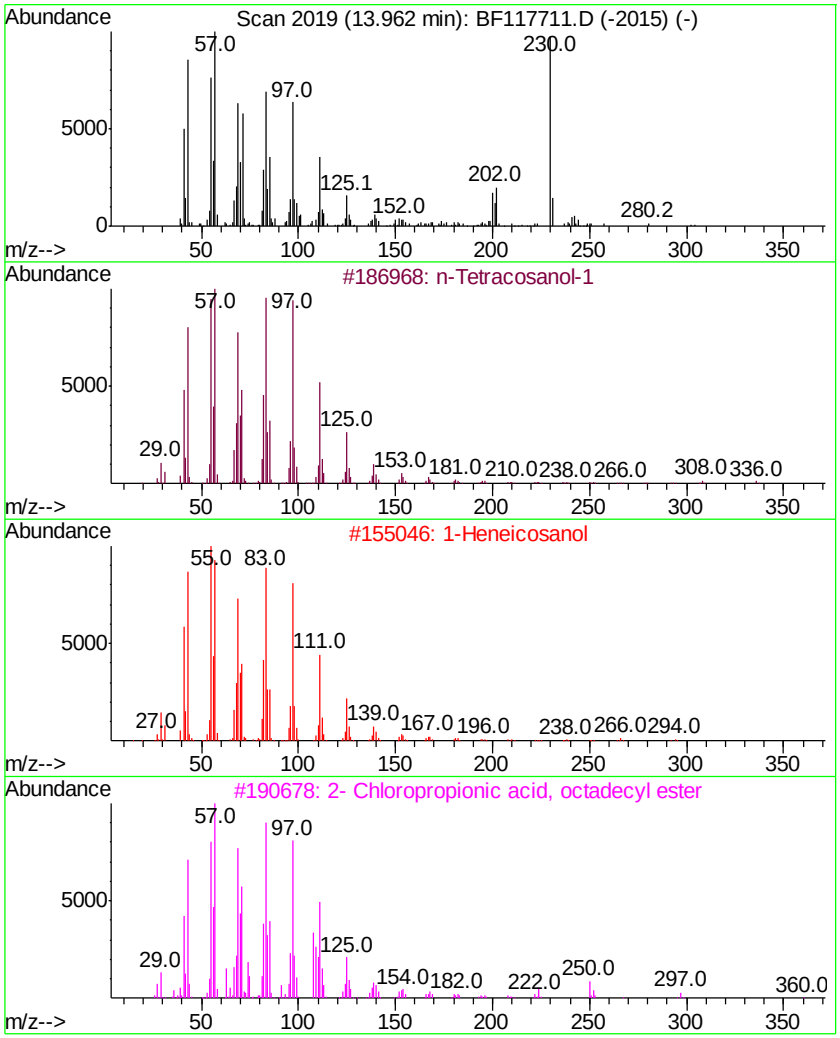
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

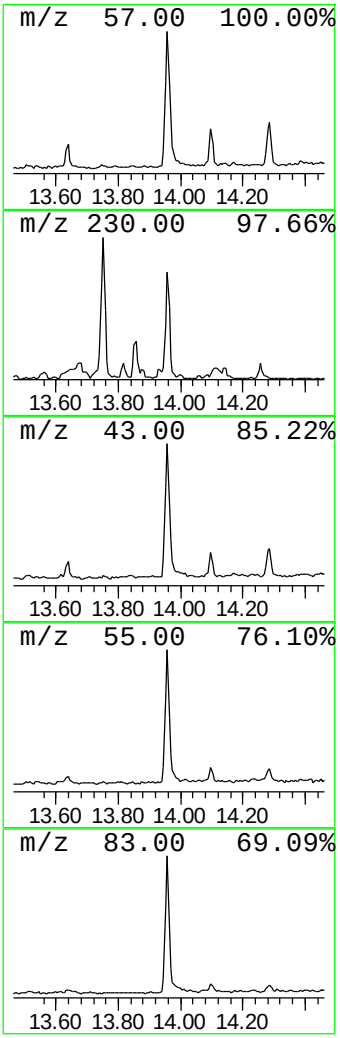
****

Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.29 ng	654520	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

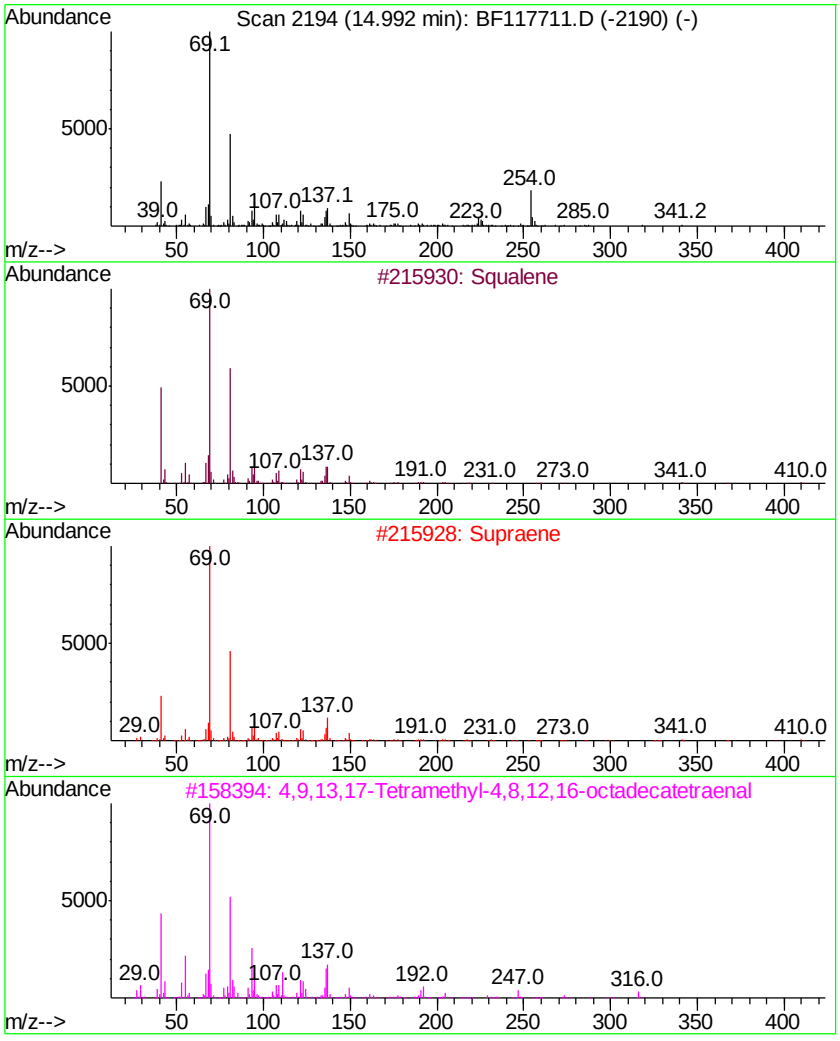
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

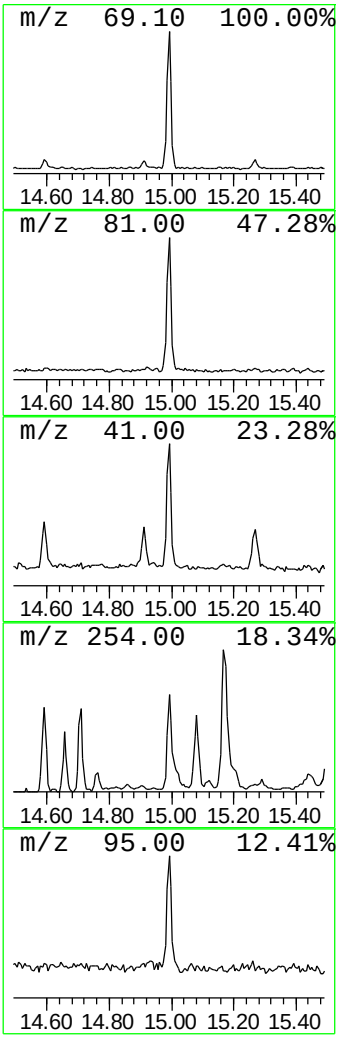
****

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.34 ng	408450	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	81
2	Supraene	410	C30H50	007683-64-9	81
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
5	Farnesol isomer a	222	C15H26O	1000108-92-4	62





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

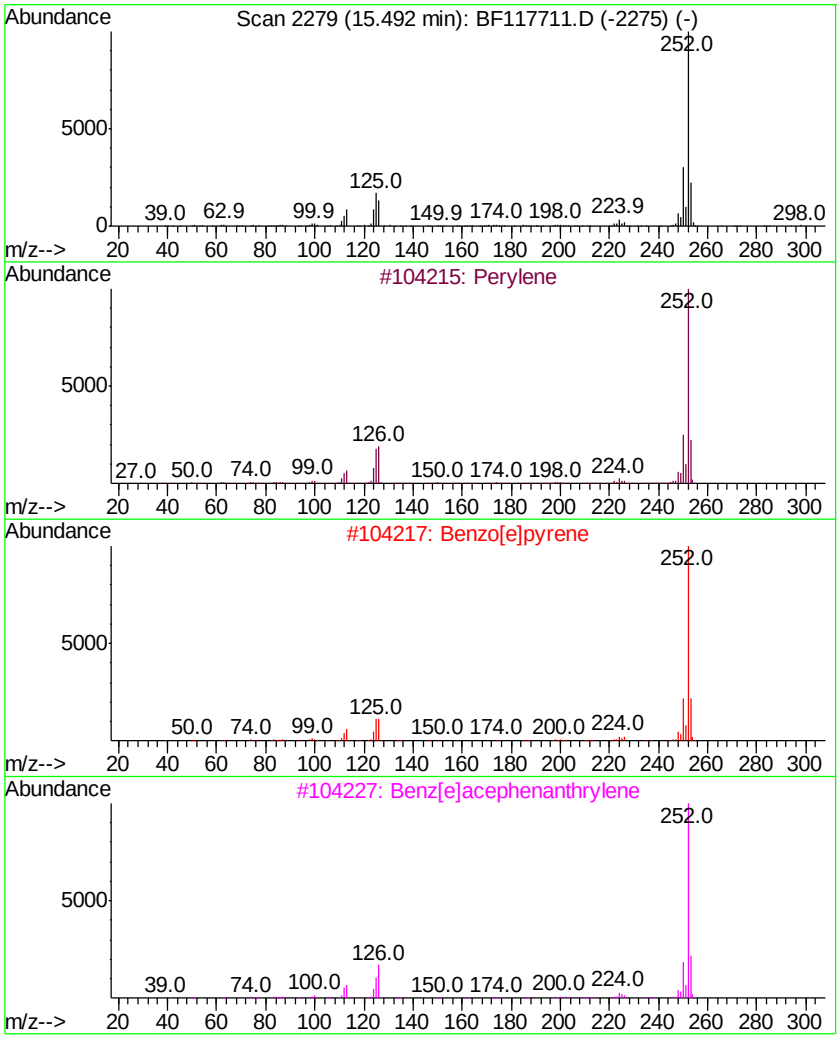
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

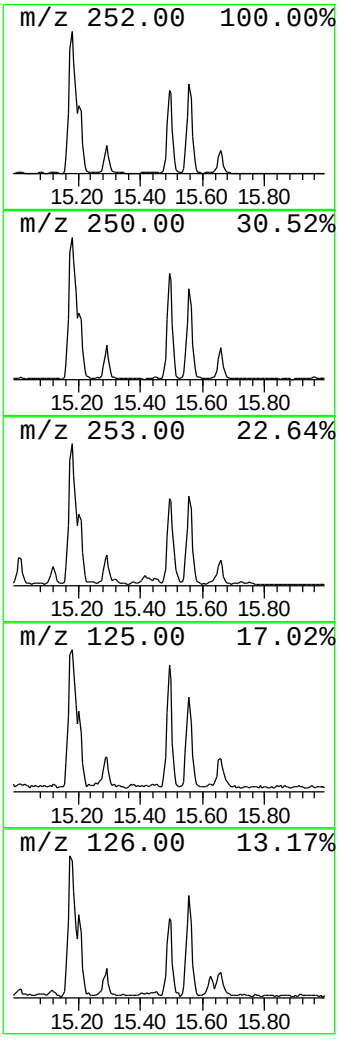
****

Peak Number 9 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	3.79 ng	463790	Perylene-d12	15.63

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	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110719\
Data File : BF117711.D
Acq On : 7 Nov 2019 18:13
Operator : JU
Sample : K5723-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 8-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	16.9	ng	1597650	1	6.93	1891790	20.0
2-Pentanone, 4-hy...	5.15	13.2	ng	1245860	1	6.93	1891790	20.0
unknown6.70	6.70	61.6	ng	5830580	1	6.93	1891790	20.0
n-Hexadecanoic acid	11.99	4.0	ng	591063	4	11.47	2976920	20.0
n-Tetracosanol-1	13.96	4.3	ng	654520	5	14.12	3047940	20.0
Squalene	14.99	3.3	ng	408450	6	15.63	2448310	20.0
Perylene	15.49	3.8	ng	463790	6	15.63	2448310	20.0