LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102017\
Data File : BF099707.D
Acq On : 20 Oct 2017 18:10
Operator : SJ/JU
Sample : I5981-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	5.022	497	499	516	rBB	37923	50353	6.29%	0.566%
2	5.434	566	569	582	rBV	295768	341077	42.64%	3.833%
3	6.451	739	742	761	rBV	328547	365104	45.64%	4.103%
4	6.581	761	764	773	rVB	418766	398146	49.77%	4.474%
5	6.810	800	803	814	rBB	579401	497594	62.21%	5.591%
6	6.969	826	830	840	rVB	334778	301800	37.73%	3.391%
7	7.375	897	899	908	rBV	220841	213815	26.73%	2.403%
8	8.092	1018	1021	1027	rBV	809134	663364	82.93%	7.454%
9	8.375	1061	1069	1072	rBV3	7017	11412	1.43%	0.128%
10	8.751	1129	1133	1139	rVB6	4823	10188	1.27%	0.114%
11	8.910	1158	1160	1162	rVB2	12633	10234	1.28%	0.115%
12	9.163	1200	1203	1208	rBV	570094	435911	54.49%	4.898%
13	9.239	1212	1216	1219	rBV	18310	17402	2.18%	0.196%
14	9.563	1265	1271	1273	rBV4	14169	18967	2.37%	0.213%
15	9.710	1292	1296	1299	rBV3	8797	10216	1.28%	0.115%
16	9.769	1303	1306	1309	rVB	21452	20033	2.50%	0.225%
17	9.845	1316	1319	1323	rVB2	757303	624411	78.06%	7.016%
18	10.086	1358	1360	1364	rVB4	7759	9175	1.15%	0.103%
19	10.263	1384	1390	1393	rBV	27710	26393	3.30%	0.297%
20	10.486	1421	1428	1430	rBV3	10744	15631	1.95%	0.176%
21	10.639	1450	1454	1462	rBV	170767	162086	20.26%	1.821%
22	10.739	1467	1471	1479	rVV	31089	37220	4.65%	0.418%
23	11.186	1544	1547	1549	rBV	26266	21007	2.63%	0.236%
24	11.216	1549	1552	1554	rVV2	11446	9866	1.23%	0.111%
25	11.333	1569	1572	1575	rBV	613956	494036	61.76%	5.551%
26	11.357	1575	1576	1580	rVV	45033	30542	3.82%	0.343%
27	11.416	1583	1586	1590	rVB	12045	11754	1.47%	0.132%
28	11.610	1617	1619	1625	rBV	23952	19690	2.46%	0.221%
29	11.716	1633	1637	1640	rBV	306845	246391	30.80%	2.769%
30	11.851	1655	1660	1661	rBV2	10343	13950	1.74%	0.157%
31	11.868	1661	1663	1668	rVB4	10834	10527	1.32%	0.118%
32	11.951	1674	1677	1679	rBV2	10994	11226	1.40%	0.126%
33	12.016	1685	1688	1694	rVB	20678	18581	2.32%	0.209%
34	12.398	1749	1753	1755	rBV	910527	799923	100.00%	8.989%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102017\
Data File : BF099707.D
Acq On : 20 Oct 2017 18:10
Operator : SJ/JU
Sample : I5981-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.421	1755	1757	1763	rVB	761238	638238	79.79%	7.172%
36	12.504	1768	1771	1774	rVB	136769	100072	12.51%	1.125%
37	12.551	1775	1779	1783	rBV	91235	89839	11.23%	1.010%
38	12.739	1806	1811	1813	rBV2	18168	18643	2.33%	0.209%
39	12.780	1813	1818	1824	rVB	92709	93355	11.67%	1.049%
40	12.910	1837	1840	1844	rVB	327530	280891	35.11%	3.156%
41	12.992	1851	1854	1858	rBV5	6292	9736	1.22%	0.109%
42	13.063	1864	1866	1868	rBV3	16239	13395	1.67%	0.151%
43	13.092	1868	1871	1872	rVV2	8976	11631	1.45%	0.131%
44	13.110	1872	1874	1876	rVB	14643	12104	1.51%	0.136%
45	13.227	1889	1894	1896	rBV4	17171	18975	2.37%	0.213%
46	13.339	1910	1913	1918	rBV6	11711	14913	1.86%	0.168%
47	13.474	1932	1936	1940	rBV3	11211	13439	1.68%	0.151%
48	13.798	1989	1991	1996	rBV3	28082	33139	4.14%	0.372%
49	13.898	2005	2008	2011	rBV3	13876	15771	1.97%	0.177%
50	13.974	2017	2021	2025	rBV	574782	571684	71.47%	6.424%
51	14.004	2025	2026	2029	rVB	42295	22769	2.85%	0.256%
52	14.209	2057	2061	2064	rBV6	8796	14121	1.77%	0.159%
53	14.404	2090	2094	2095	rBV3	9897	11970	1.50%	0.135%
54	14.421	2095	2097	2100	rVV4	12695	16920	2.12%	0.190%
55	14.509	2110	2112	2114	rVB3	12962	9544	1.19%	0.107%
56	15.015	2195	2198	2201	rBV	39242	54622	6.83%	0.614%
57	15.045	2201	2203	2207	rVB2	49328	50728	6.34%	0.570%
58	15.121	2214	2216	2222	rVB3	14749	16070	2.01%	0.181%
59	15.315	2246	2249	2254	rVB	27034	31714	3.96%	0.356%
60	15.380	2256	2260	2263	rVV	35738	49819	6.23%	0.560%
61	15.439	2263	2270	2279	rVB	422781	579747	72.48%	6.515%
62	15.839	2334	2338	2344	rBV2	41954	60247	7.53%	0.677%
63	16.333	2417	2422	2426	rBV3	21780	32952	4.12%	0.370%
64	16.509	2450	2452	2456	rVB4	10940	12685	1.59%	0.143%
65	16.903	2513	2519	2526	rVB3	32550	71425	8.93%	0.803%

Sum of corrected areas: 8899183

LSC Report - Integrated Chromatogram

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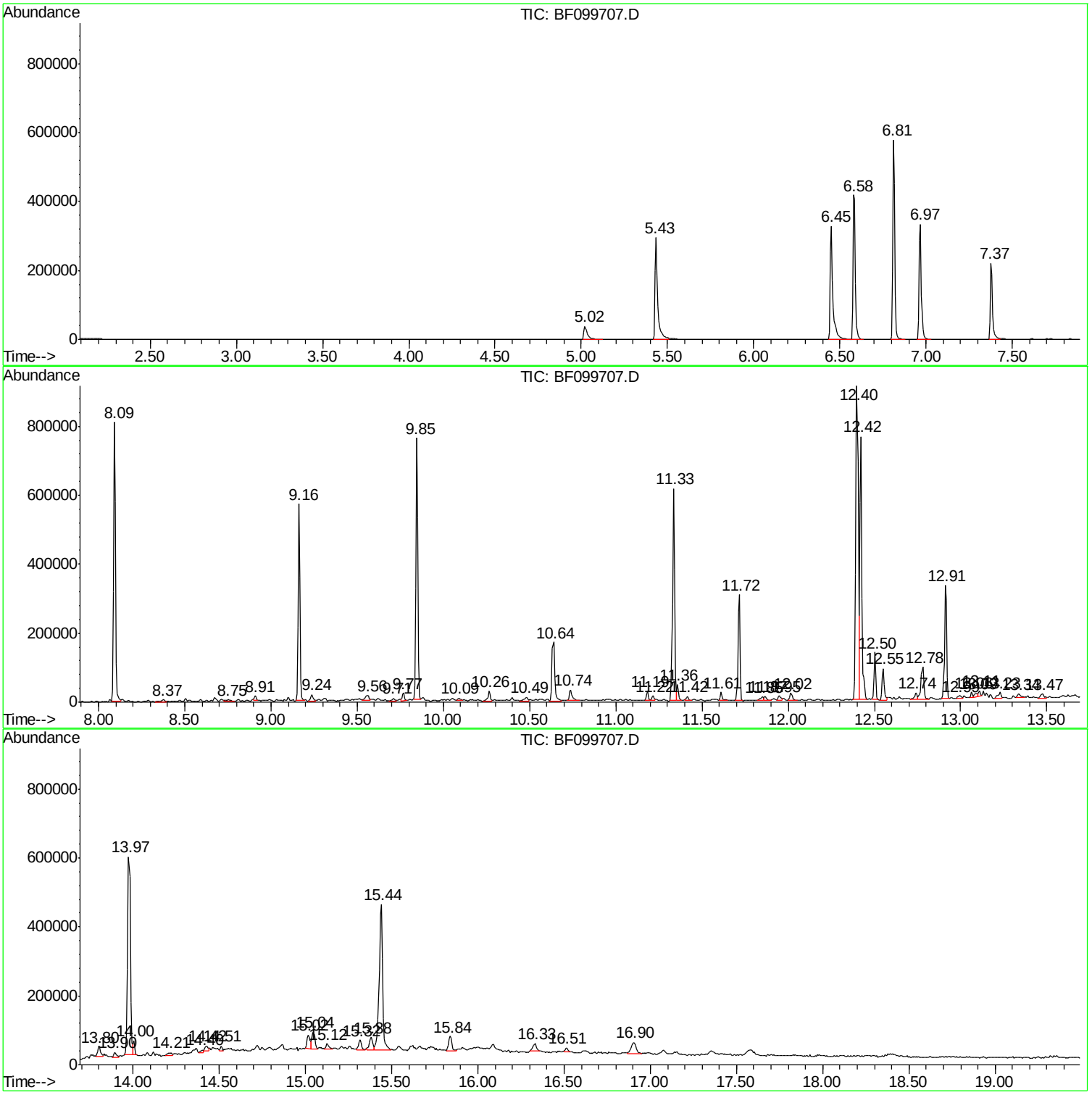
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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TIC Integration Parameters: LSCINT.P

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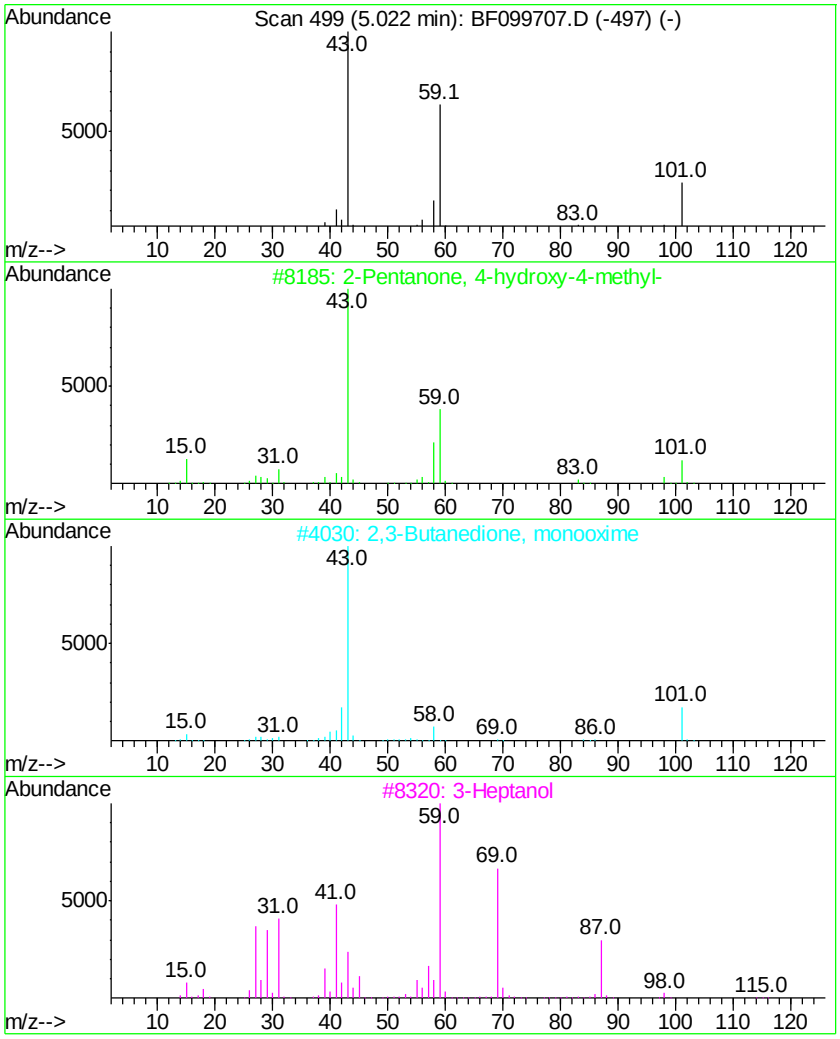
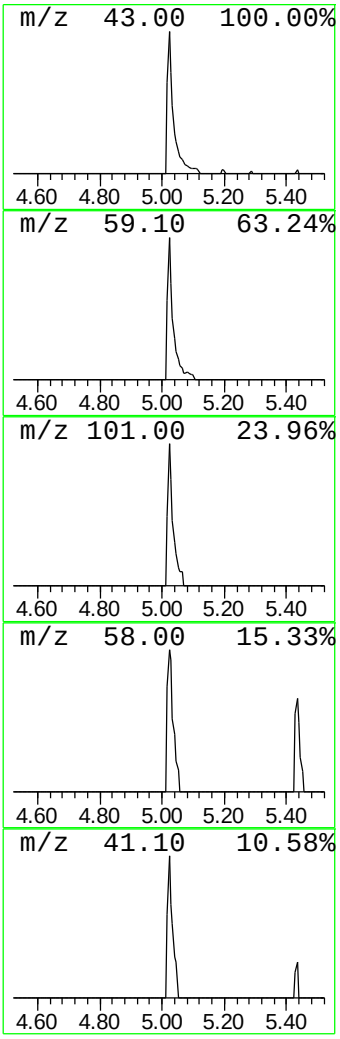
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.02 ng	50353	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	3-Heptanol	116	C7H16O	000589-82-2	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

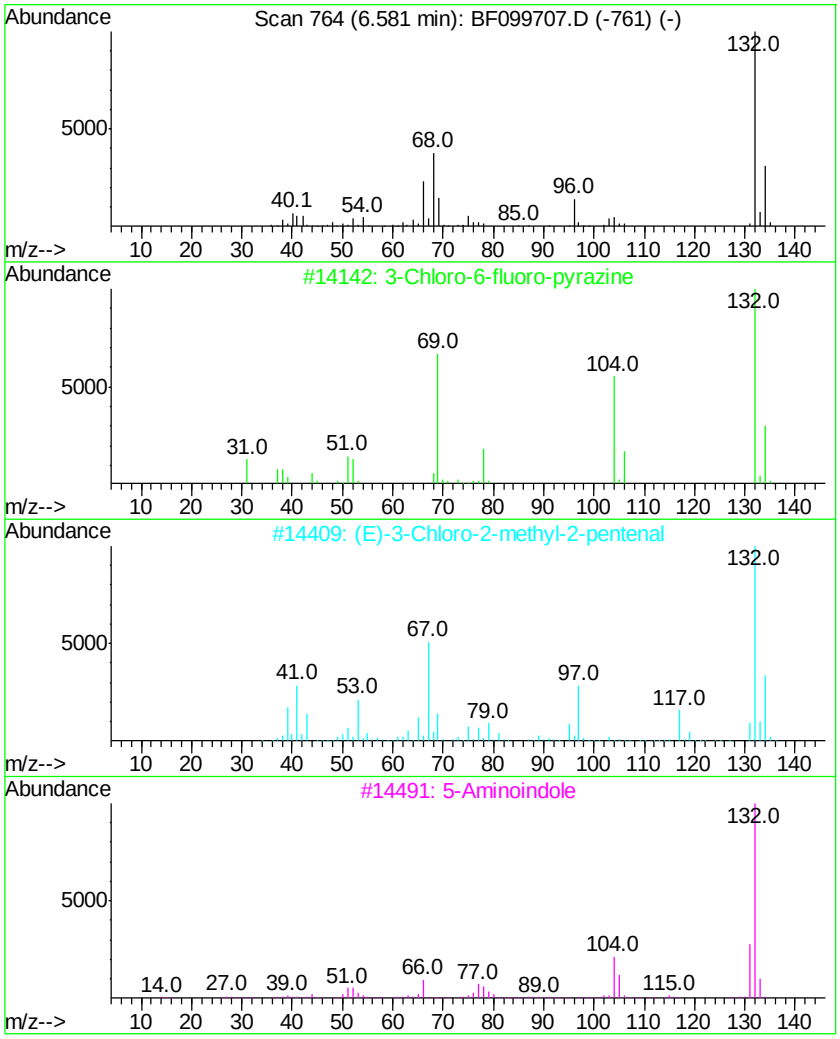
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

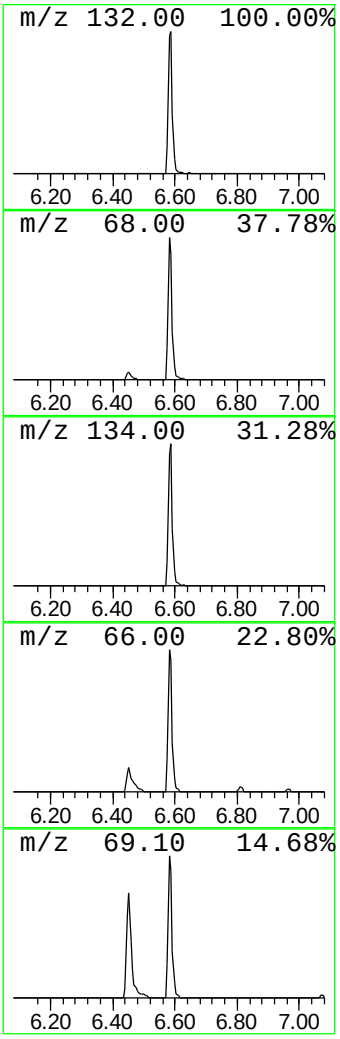
****

Peak Number 2 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	16.00 ng	398146	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Sample : I5981-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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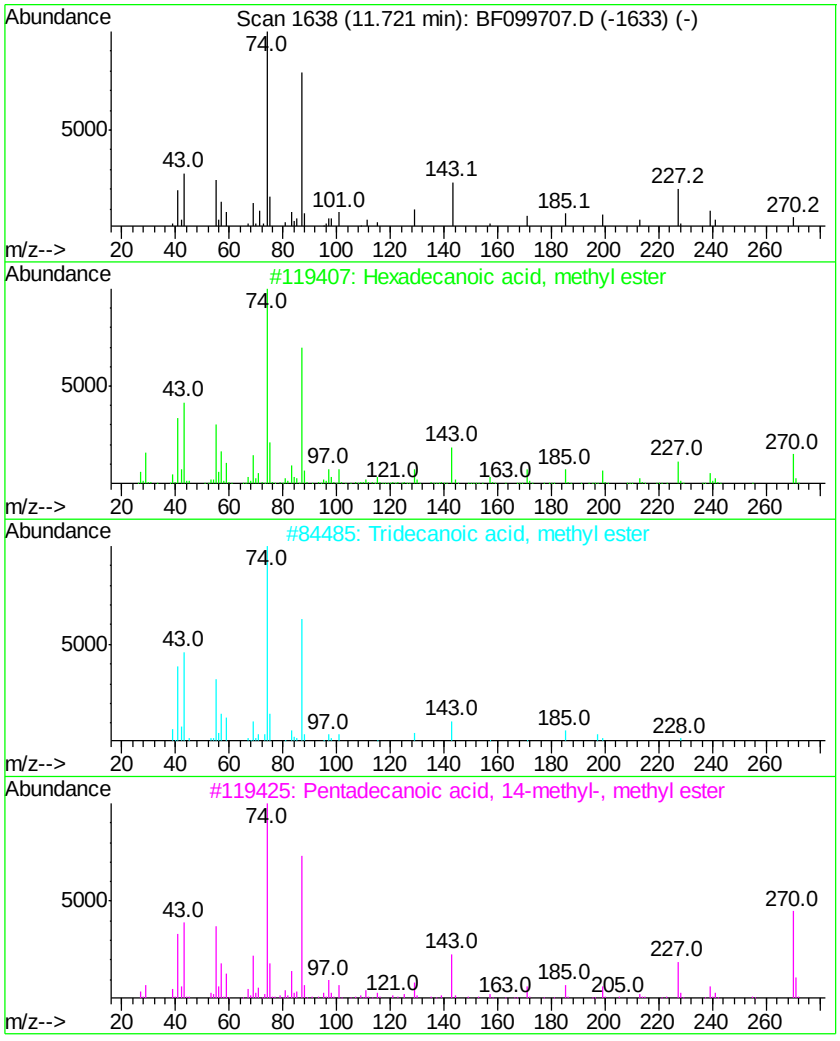
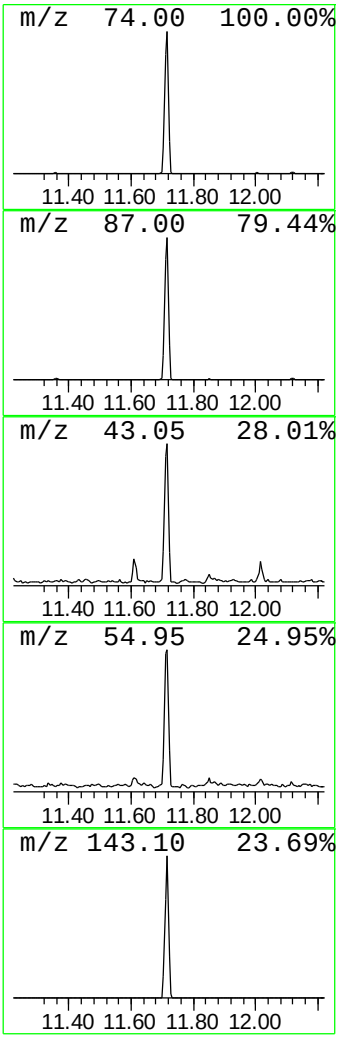
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	9.97 ng	246391	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	92
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	89
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80





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Misc :
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Instrument : BNA_F
ClientSampleId : NB-01-101817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Integration Parameters: LSCINT.P

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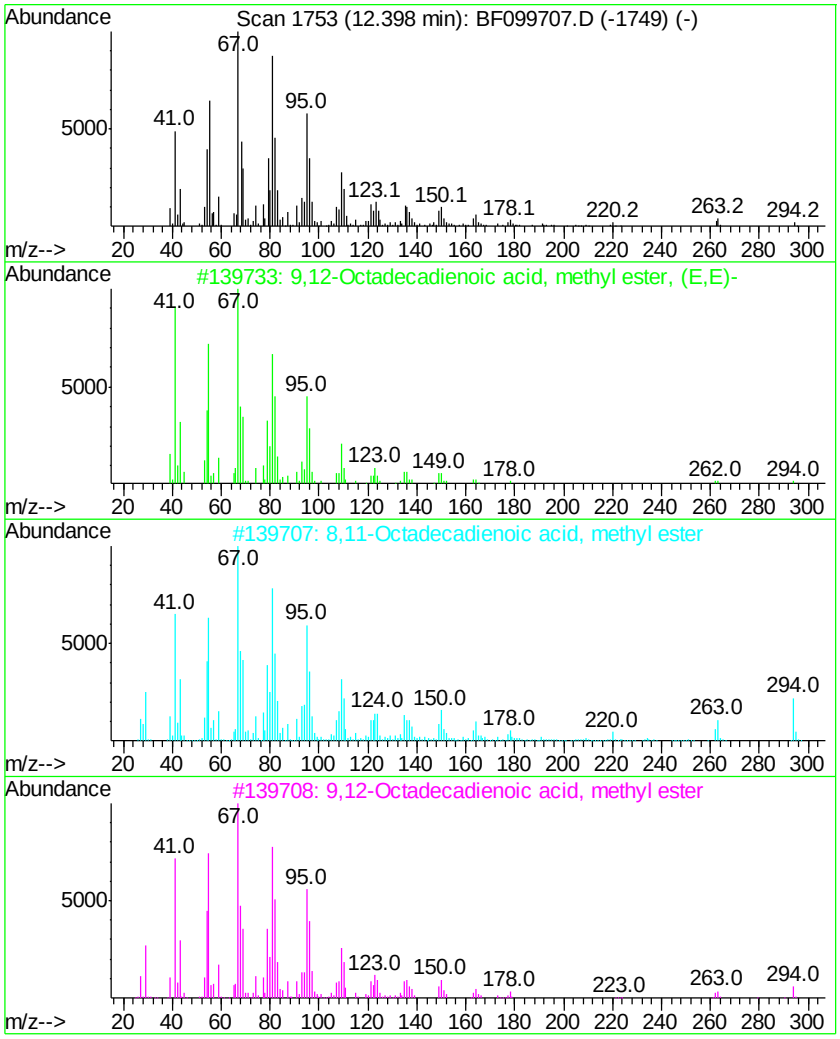
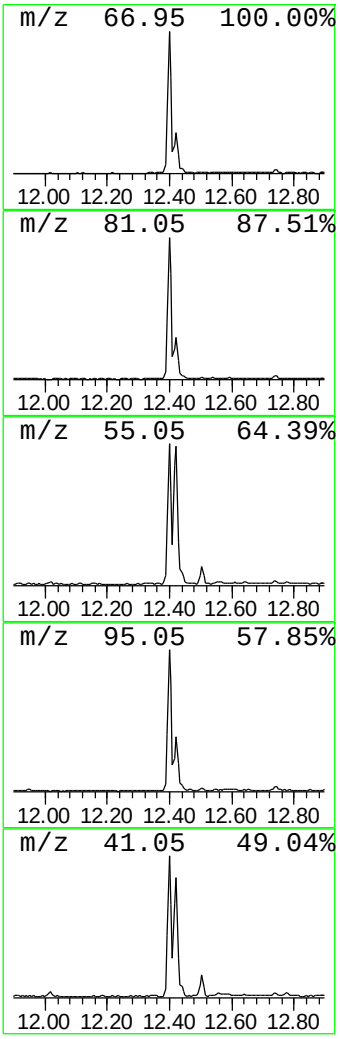
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	32.38 ng	799923	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





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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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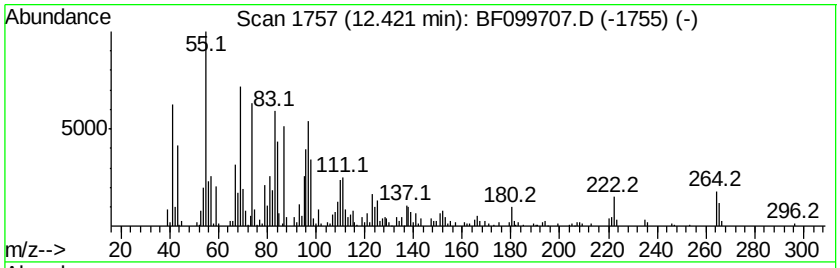
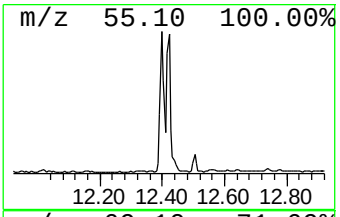
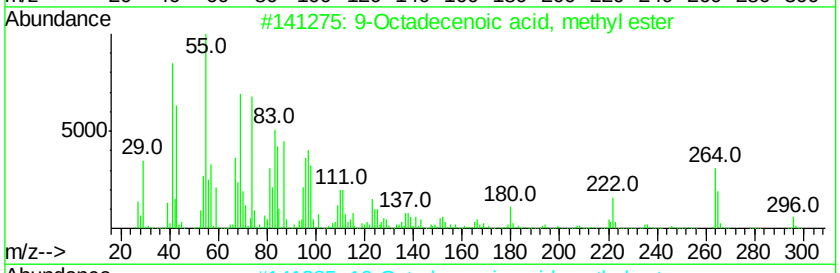
Peak Number 6 9-Octadecenoic acid, methyl... Concentration Rank 2

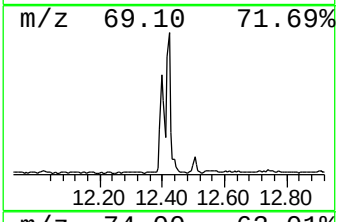
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	25.84 ng	638238	Phenanthrene-d10	11.33

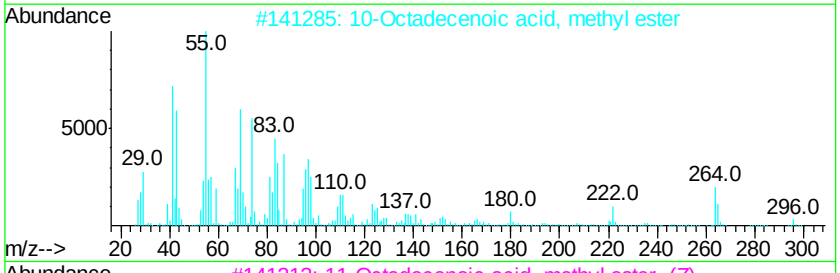
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99

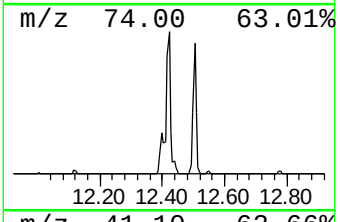


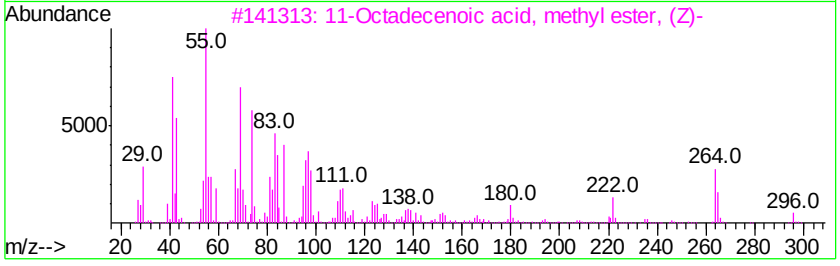


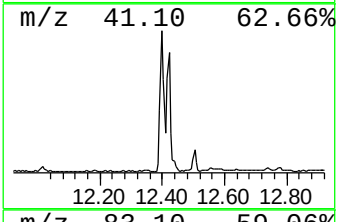


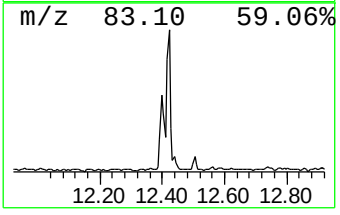












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

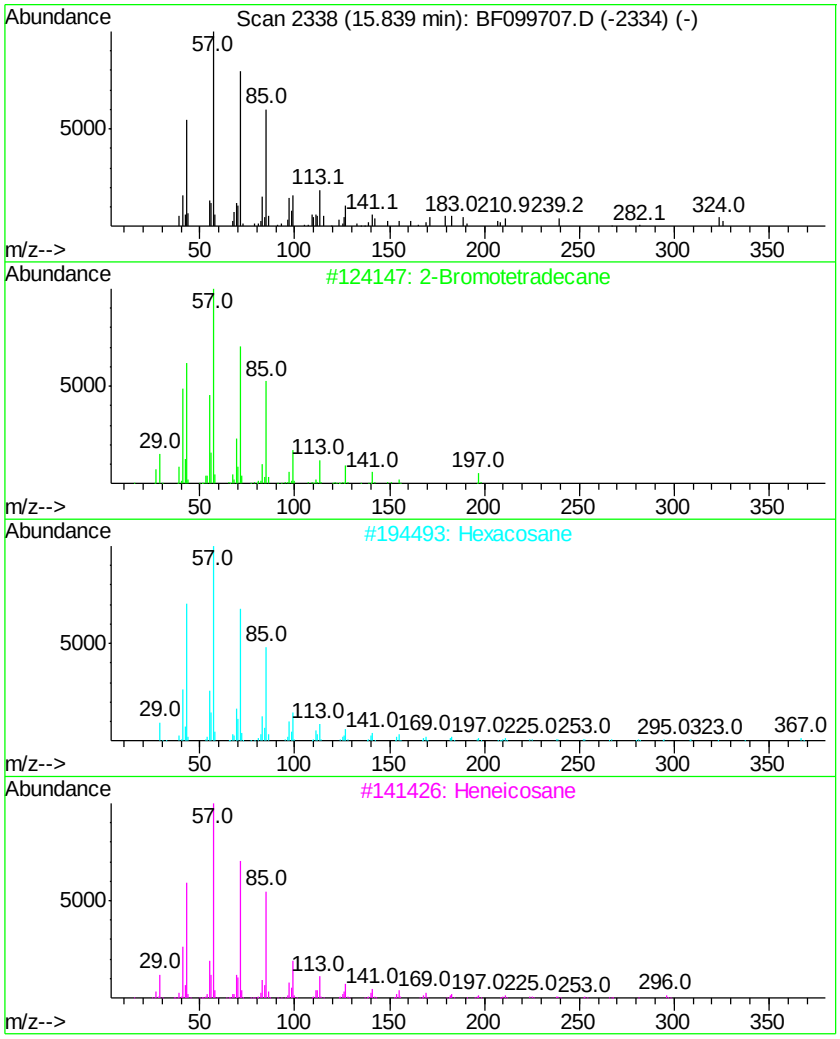
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

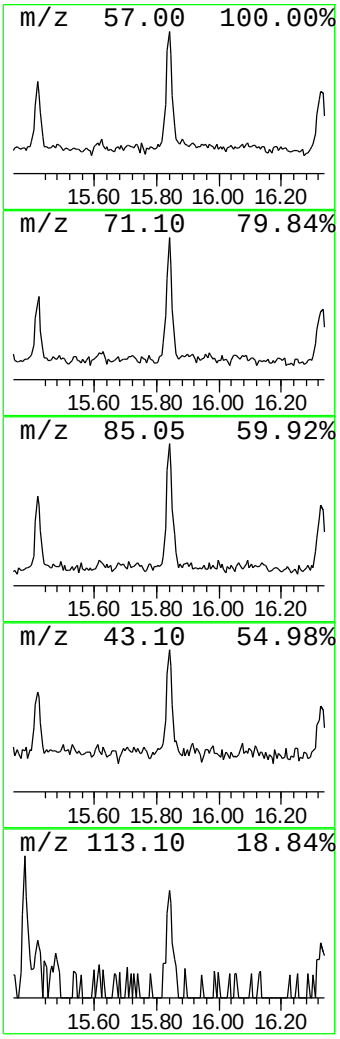
****

Peak Number 7 2-Bromotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.08 ng	60247	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
2	Hexacosane	366	C26H54	000630-01-3	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Eicosane	282	C20H42	000112-95-8	72
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102017\
Data File : BF099707.D
Acq On : 20 Oct 2017 18:10
Operator : SJ/JU
Sample : I5981-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-101817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.02	2.0	ng	50353	1	6.81	497594	20.0
unknown6.58	6.58	16.0	ng	398146	1	6.81	497594	20.0
Hexadecanoic acid...	11.72	10.0	ng	246391	4	11.33	494036	20.0
9,12-Octadecadien...	12.40	32.4	ng	799923	4	11.33	494036	20.0
9-Octadecenoic ac...	12.42	25.8	ng	638238	4	11.33	494036	20.0
2-Bromotetradecane	15.84	2.1	ng	60247	6	15.44	579747	20.0