LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

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-BF040618.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	3.840	293	298	306	rVB	67691	94208	3.37%	0.335%
2	5.016	491	498	506	rBV	121403	161790	5.79%	0.576%
3	5.275	539	542	546	rBV	57226	56863	2.03%	0.202%
4	5.387	557	561	562	rBV	134511	133396	4.77%	0.475%
5	5.422	562	567	570	rVB	2767831	2666326	95.38%	9.490%
6	5.645	602	605	610	rBV	56716	52652	1.88%	0.187%
7	6.257	707	709	713	rBV	60103	48761	1.74%	0.174%
8	6.322	718	720	723	rBV	109378	89357	3.20%	0.318%
9	6.357	723	726	729	rBV	54133	42634	1.53%	0.152%
10	6.398	729	733	735	rBV2	51951	44496	1.59%	0.158%
11	6.439	735	740	743	rVV	2328045	2624879	93.90%	9.343%
12	6.487	745	748	754	rVV	35610	40253	1.44%	0.143%
13	6.575	758	763	766	rVV	3066192	2715871	97.15%	9.667%
14	6.628	769	772	776	rVB	200439	169262	6.05%	0.602%
15	6.804	798	802	805	rBV	931652	759322	27.16%	2.703%
16	6.957	824	828	831	rBV	2409508	2244428	80.29%	7.989%
17	6.981	831	832	835	rVB	84620	46610	1.67%	0.166%
18	7.045	841	843	846	rBV	44227	40339	1.44%	0.144%
19	7.075	846	848	851	rVV	42218	33304	1.19%	0.119%
20	7.122	852	856	863	rVB	91015	96162	3.44%	0.342%
21	7.334	889	892	894	rBV	104231	96693	3.46%	0.344%
22	7.369	894	898	901	rVB	1882451	1663841	59.52%	5.922%
23	7.757	961	964	968	rVB2	34626	33489	1.20%	0.119%
24	7.822	968	975	977	rBV2	51981	51518	1.84%	0.183%
25	8.086	1016	1020	1023	rBV	1143415	934247	33.42%	3.325%
26	9.163	1198	1203	1206	rBV	3247244	2795469	100.00%	9.950%
27	9.557	1266	1270	1277	rBV	220026	224940	8.05%	0.801%
28	9.704	1291	1295	1298	rBV	31544	32790	1.17%	0.117%
29	9.769	1303	1306	1309	rVB	88501	71675	2.56%	0.255%
30	9.839	1314	1318	1322	rBV2	1053818	890884	31.87%	3.171%
31	10.269	1388	1391	1393	rVB	100132	80332	2.87%	0.286%
32	10.633	1449	1453	1458	rBV	1390558	1316225	47.08%	4.685%
33	10.739	1468	1471	1476	rBV	98857	114466	4.09%	0.407%
34	11.186	1545	1547	1550	rBV	36425	38846	1.39%	0.138%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.216	1550	1552	1558	rVB2	37230	47226	1.69%	0.168%
36	11.327	1568	1571	1574	rBV	849882	725921	25.97%	2.584%
37	11.351	1574	1575	1581	rVB	97094	68427	2.45%	0.244%
38	12.369	1745	1748	1753	rVB3	37338	53079	1.90%	0.189%
39	12.469	1762	1765	1771	rVB	42570	51662	1.85%	0.184%
40	12.545	1775	1778	1782	rVB	190348	176643	6.32%	0.629%
41	12.774	1811	1817	1822	rBV	349588	353596	12.65%	1.259%
42	12.916	1837	1841	1849	rVB	2166227	2055227	73.52%	7.315%
43	12.992	1851	1854	1860	rVB4	24950	38210	1.37%	0.136%
44	13.074	1865	1868	1870	rBV2	37203	40993	1.47%	0.146%
45	13.204	1887	1890	1893	rVB2	50018	52325	1.87%	0.186%
46	13.610	1956	1959	1964	rVB	45534	43782	1.57%	0.156%
47	13.721	1975	1978	1981	rBV2	31264	38890	1.39%	0.138%
48	13.774	1985	1987	1990	rVV2	30820	35128	1.26%	0.125%
49	13.810	1990	1993	2000	rVB2	348900	353712	12.65%	1.259%
50	13.974	2015	2021	2024	rBV2	886349	1031625	36.90%	3.672%
51	13.998	2024	2025	2031	rVB	181772	145896	5.22%	0.519%
52	14.363	2085	2087	2090	rVB2	37388	32733	1.17%	0.117%
53	14.451	2100	2102	2107	rVB4	52025	55955	2.00%	0.199%
54	14.821	2163	2165	2169	rBV3	27224	34849	1.25%	0.124%
55	15.015	2194	2198	2201	rBV	227572	315902	11.30%	1.124%
56	15.315	2246	2249	2255	rVB	109684	121330	4.34%	0.432%
57	15.374	2255	2259	2265	rVV	119385	175613	6.28%	0.625%
58	15.439	2265	2270	2284	rVB	709399	953970	34.13%	3.395%
59	15.939	2351	2355	2362	rVB3	80133	118238	4.23%	0.421%
60	16.551	2456	2459	2465	rVB8	33560	58944	2.11%	0.210%
61	16.674	2477	2480	2484	rBV4	27045	43859	1.57%	0.156%
62	16.886	2511	2516	2522	rBV2	46705	95905	3.43%	0.341%
63	17.056	2540	2545	2551	rBV6	33431	77058	2.76%	0.274%
64	17.321	2586	2590	2597	rVB2	35344	66068	2.36%	0.235%
65	17.451	2607	2612	2620	rVB2	57555	126261	4.52%	0.449%

Sum of corrected areas: 28095355

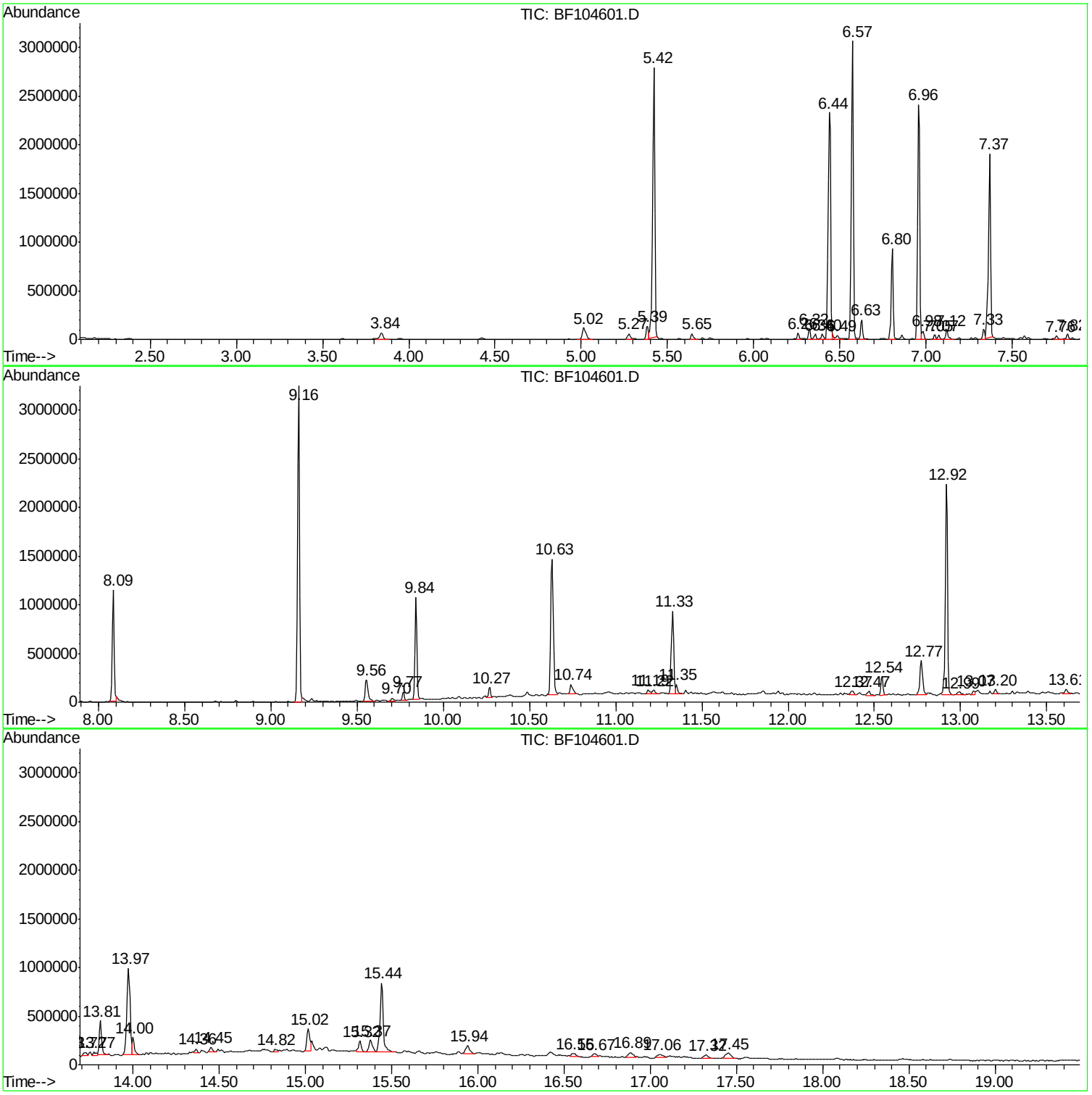
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

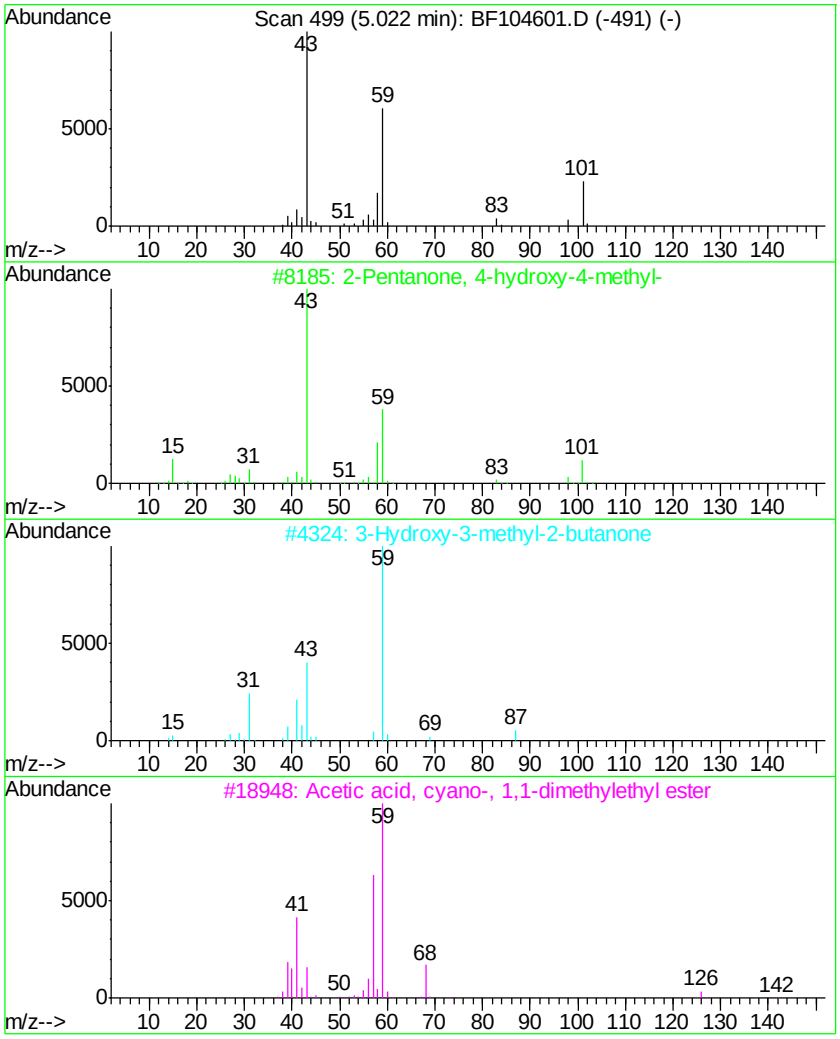
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

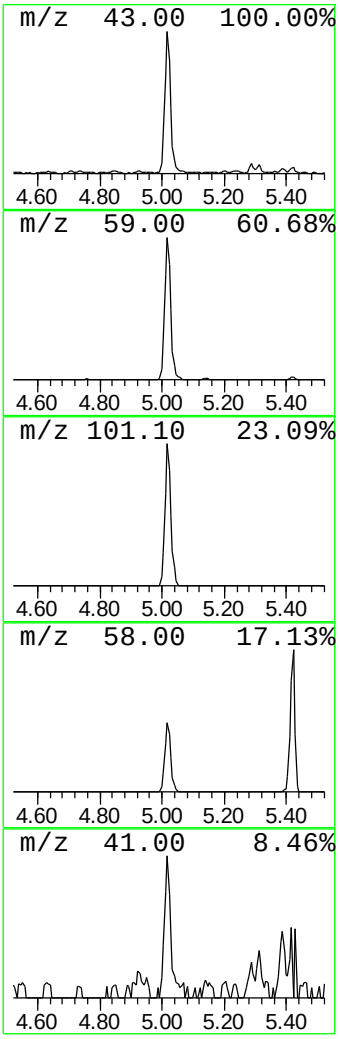
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.26 ng	161790	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

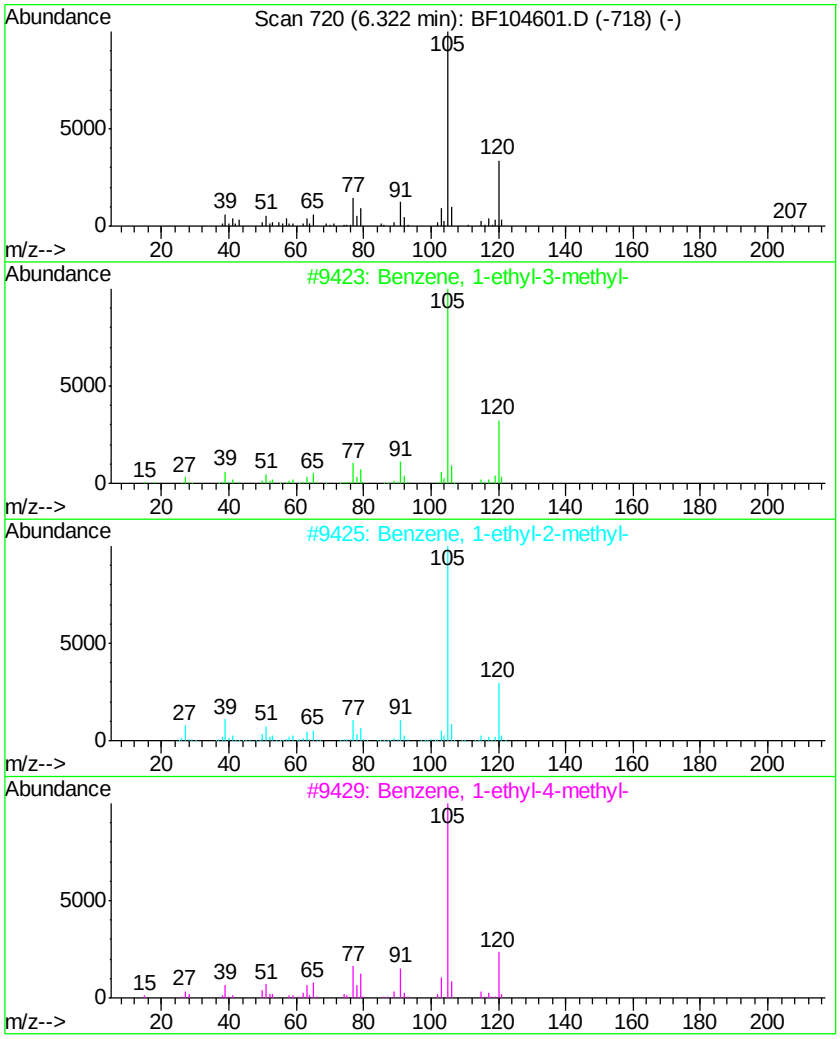
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

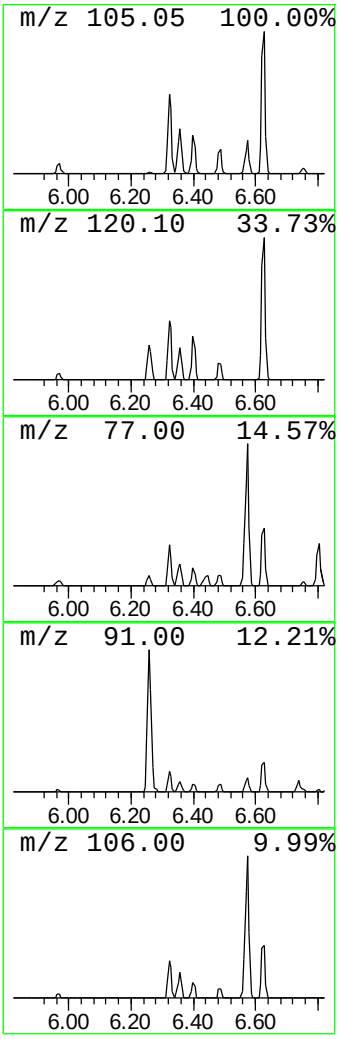
****

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	2.35 ng	89357	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

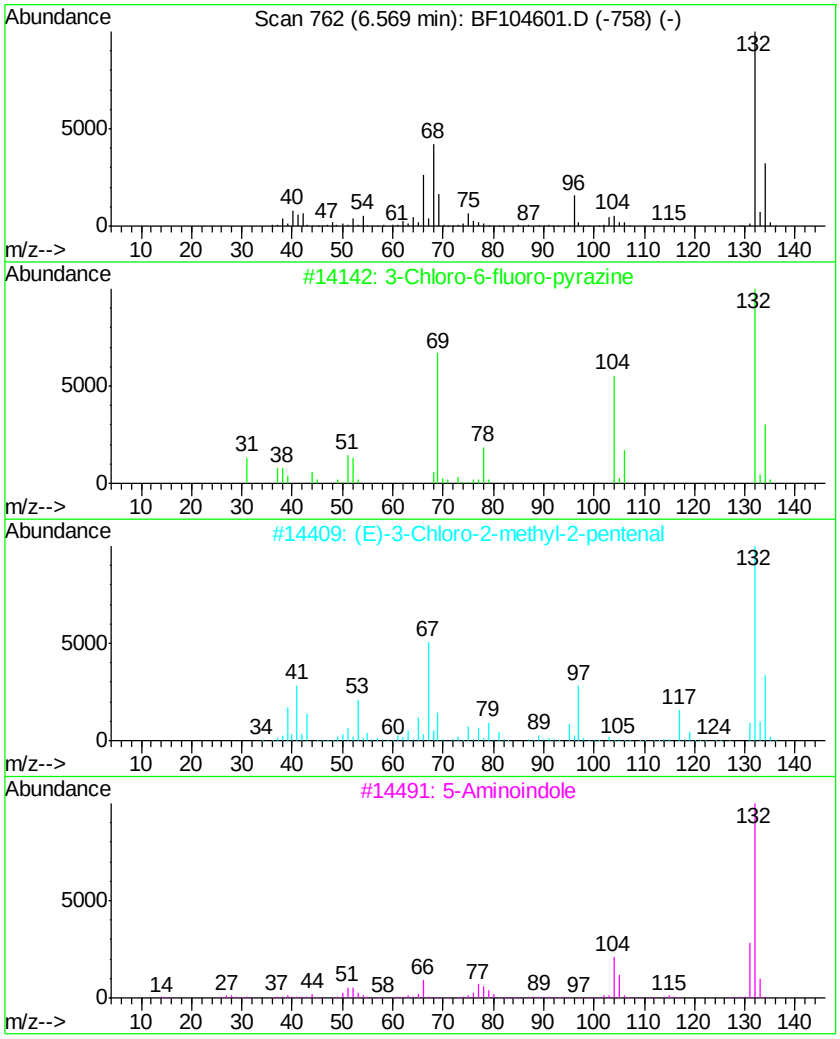
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

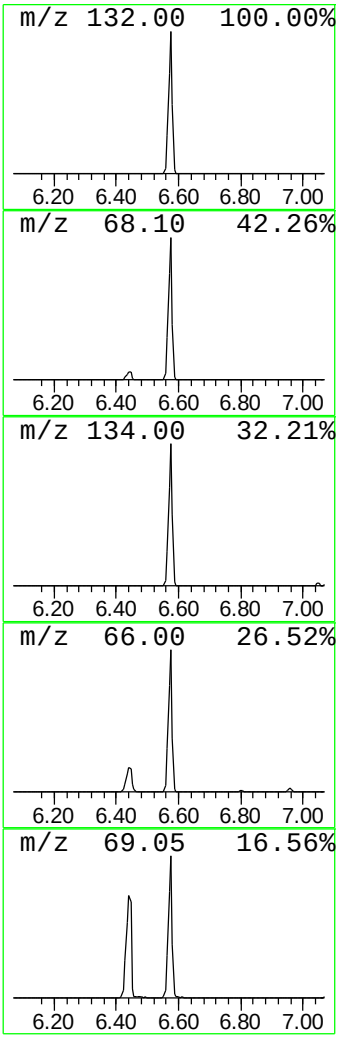
****

Peak Number 4 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.53 ng	2715870	1,4-Dichlorobenzene-d4	6.80

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	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

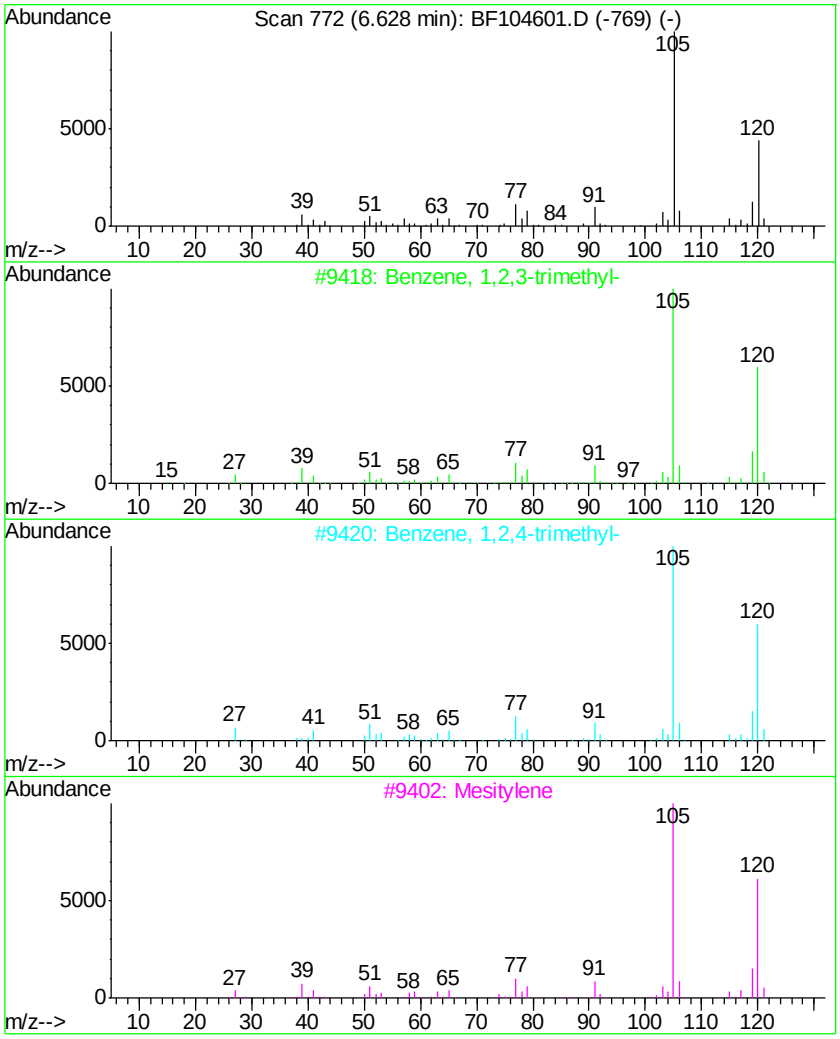
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

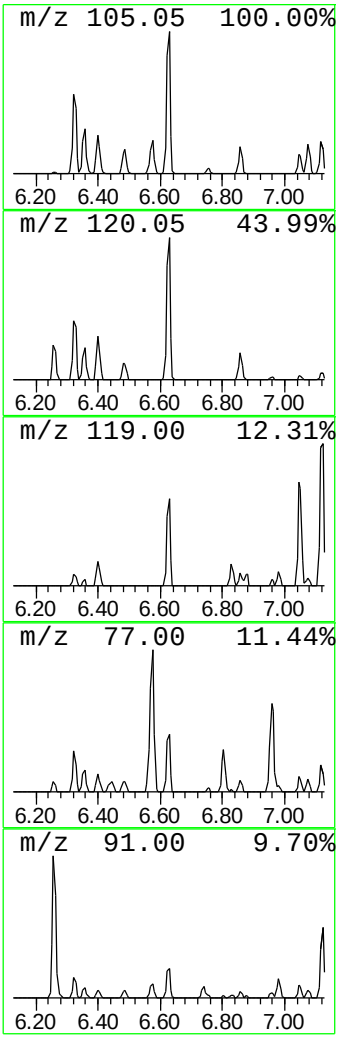
****

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	4.46 ng	169262	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Mesitylene	120	C9H12	000108-67-8	93
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

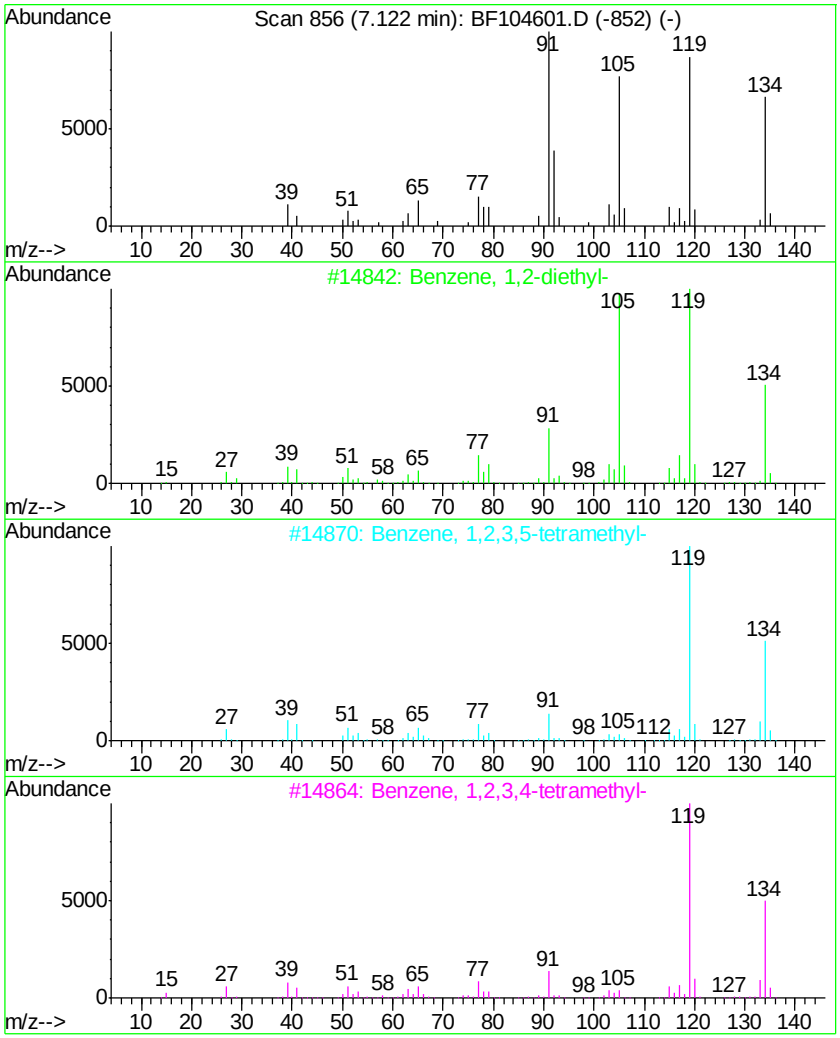
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

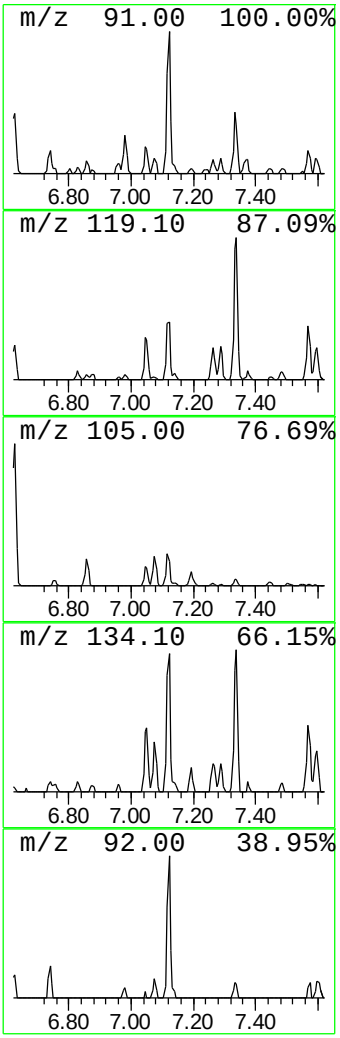
****

Peak Number 7 Benzene, 1,2-diethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	2.53 ng	96162	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
5	3a,6-Methano-3aH-indene, 2,3,4,5...	134	C10H14	098640-10-9	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

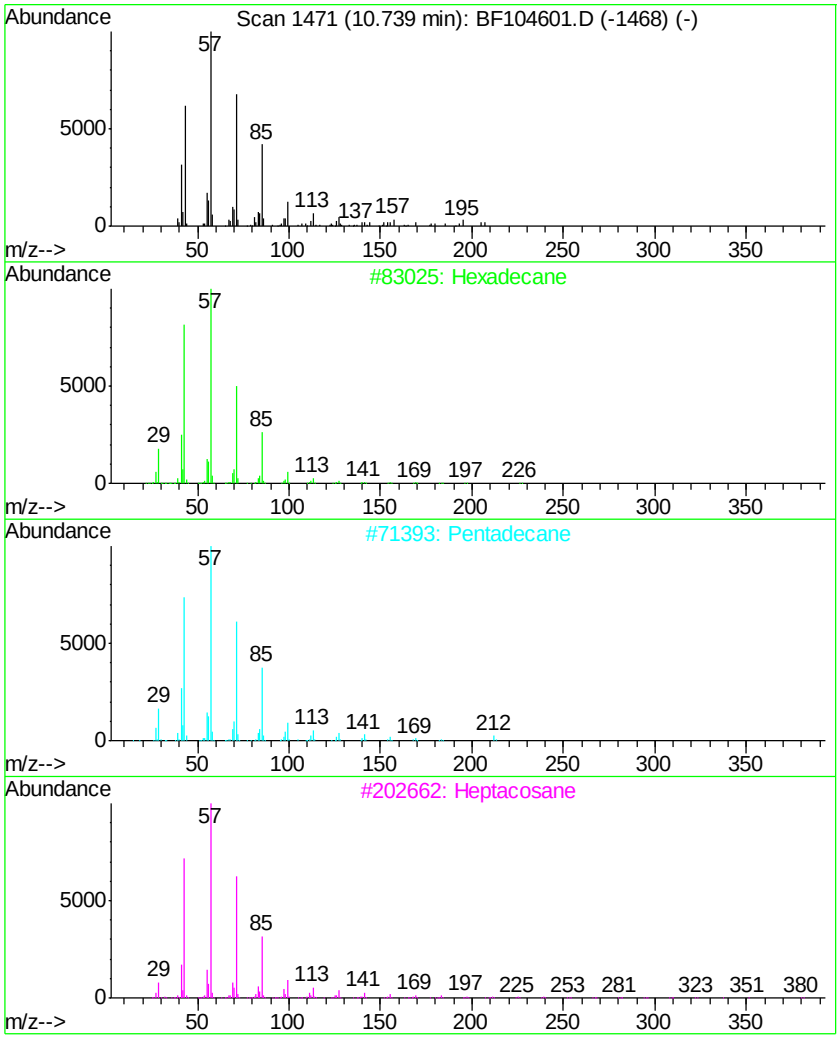
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

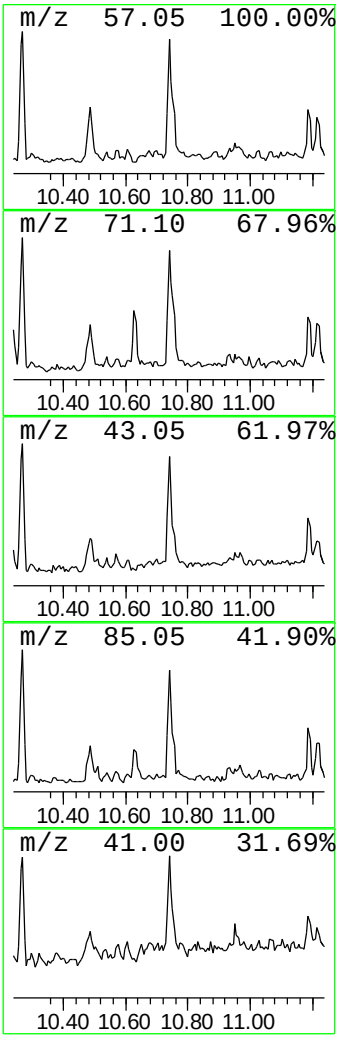
****

Peak Number 8 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	3.15 ng	114466	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane	212	C15H32	000629-62-9	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

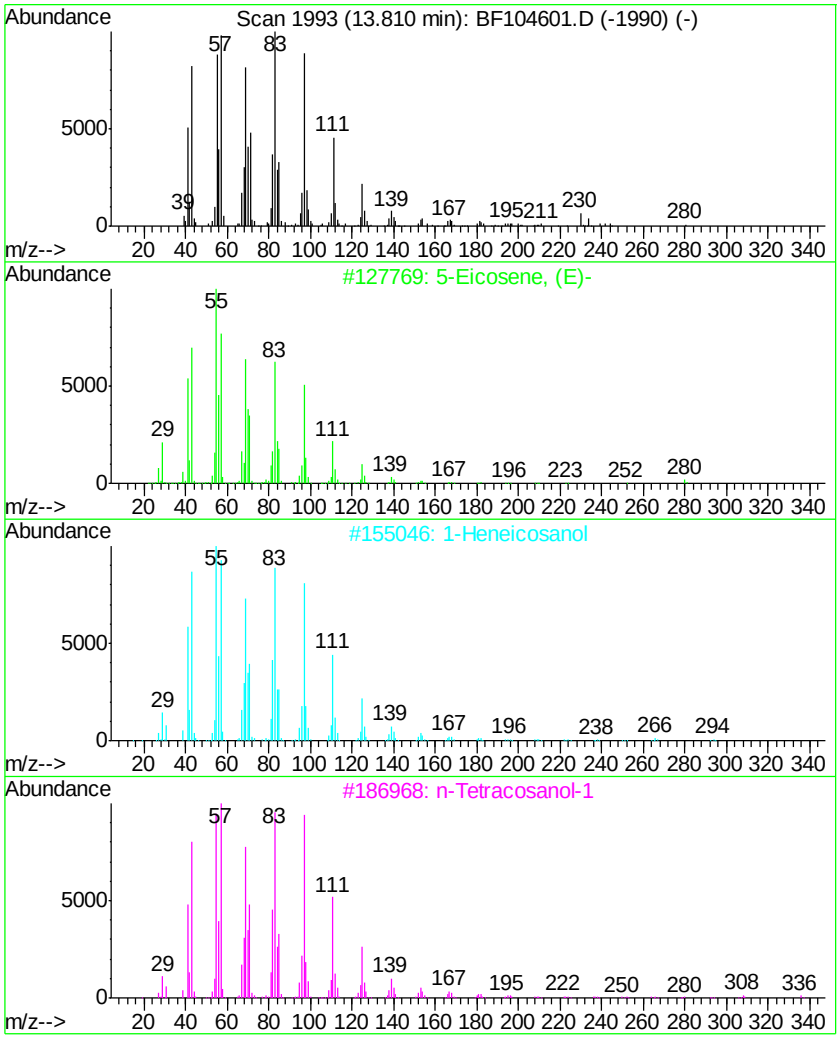
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

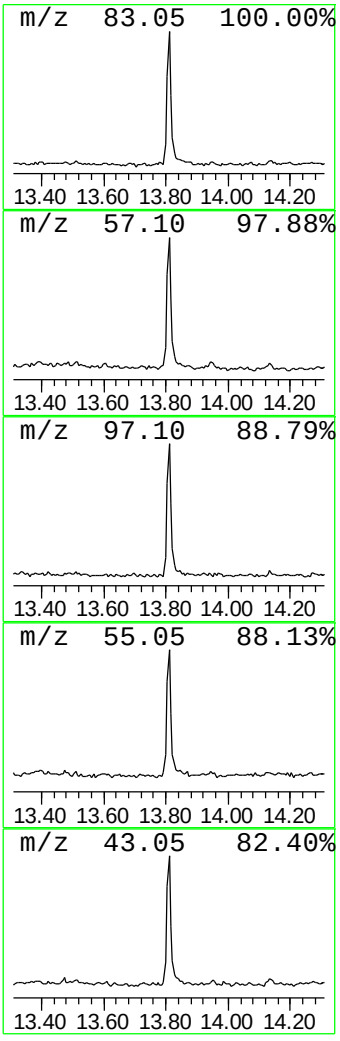
****

Peak Number 9 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.86 ng	353712	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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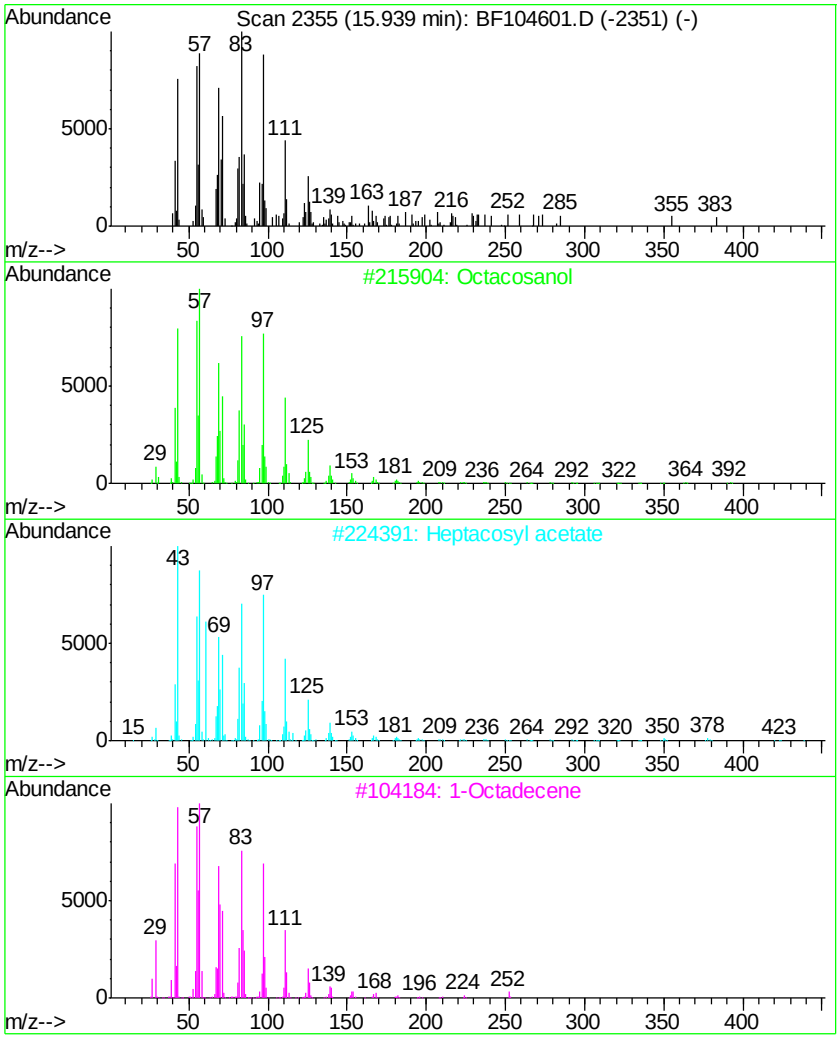
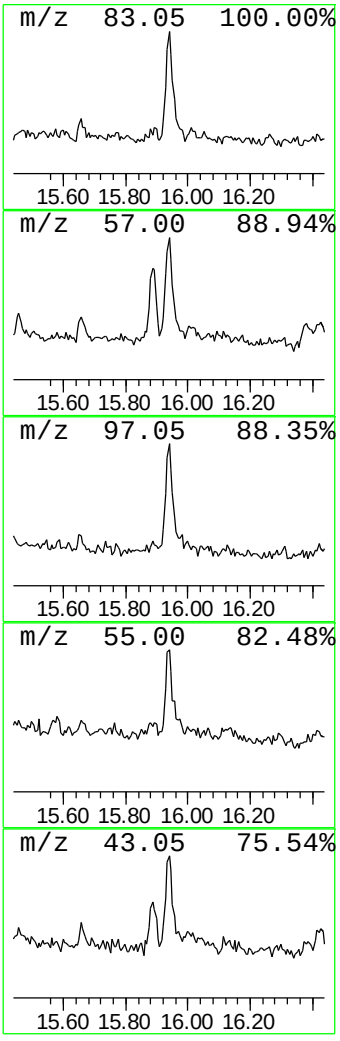
Peak Number 11 Octacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.48 ng	118238	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	93
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	93
3	1-Octadecene	252	C18H36	000112-88-9	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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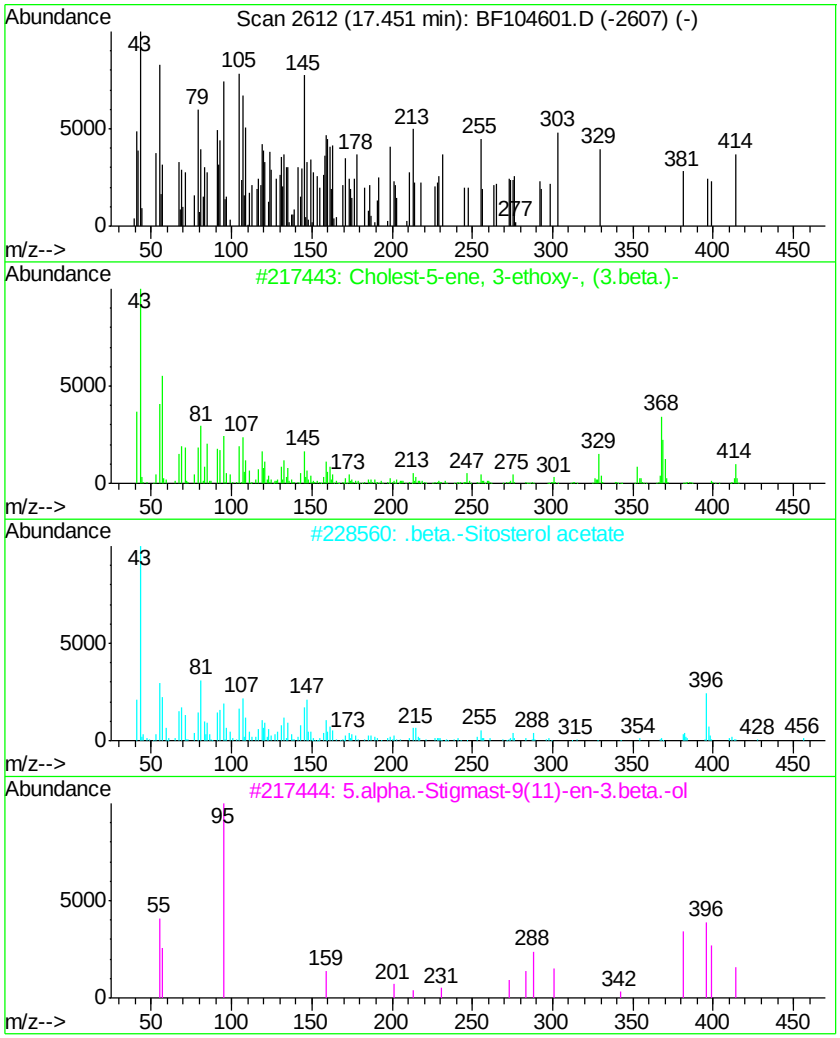
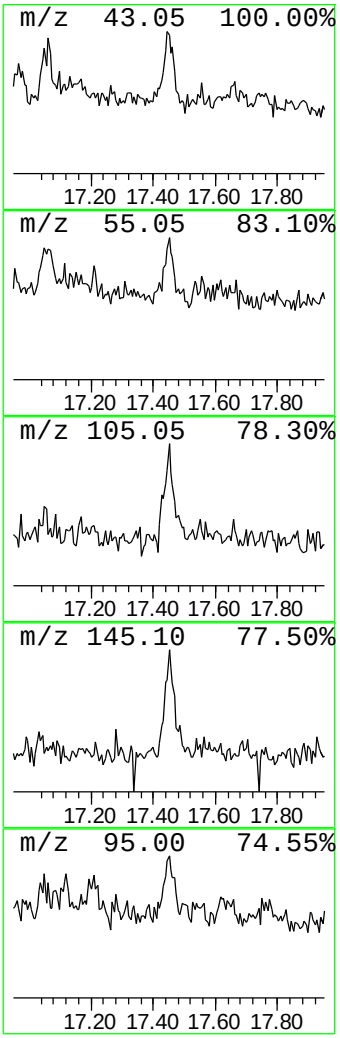
Peak Number 12 unknown17.45 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.45	2.65 ng	126261	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	45
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	22
3	5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	16
4	1H-Pyrazole-4-sulfonamide, N-(2,...	273	C10H9F2N3O2S	1000319-53-0	11
5	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041818\
Data File : BF104601.D
Acq On : 18 Apr 2018 15:04
Operator : JU/SJ
Sample : J2423-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NYS-RBR200035

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	4.3	ng	161790	1	6.80	759322	20.0
Benzene, 1-ethyl-...	6.32	2.4	ng	89357	1	6.80	759322	20.0
unknown6.57	6.57	71.5	ng	2715870	1	6.80	759322	20.0
Benzene, 1,2,3-tr...	6.63	4.5	ng	169262	1	6.80	759322	20.0
Benzene, 1,2-diet...	7.12	2.5	ng	96162	1	6.80	759322	20.0
Hexadecane	10.74	3.1	ng	114466	4	11.33	725921	20.0
5-Eicosene, (E)-	13.81	6.9	ng	353712	5	13.97	1031630	20.0
Octacosanol	15.94	2.5	ng	118238	6	15.44	953970	20.0
unknown17.45	17.45	2.6	ng	126261	6	15.44	953970	20.0