LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

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_G\METHODS\8270-BG123019.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	3.152	5	11	27	rVB	326379	590468	11.32%	1.080%
2	3.681	97	101	111	rBV	30077	54246	1.04%	0.099%
3	5.074	331	338	349	rBV	525014	830562	15.93%	1.520%
4	5.544	411	418	433	rBV	2212902	3592545	68.88%	6.573%
5	7.130	680	688	700	rBV	2295091	4182720	80.20%	7.652%
6	7.500	742	751	761	rBV	2286812	4029326	77.26%	7.372%
7	7.964	823	830	837	rBV	606795	1031206	19.77%	1.887%
8	8.287	877	885	893	rBV	1650086	2934009	56.26%	5.368%
9	9.116	1018	1026	1037	rBV	1358956	2460527	47.18%	4.502%
10	10.767	1296	1307	1314	rBV	806694	1487368	28.52%	2.721%
11	13.217	1717	1724	1733	rBV	2973816	4656613	89.29%	8.519%
12	13.499	1766	1772	1777	rBV	67969	111238	2.13%	0.204%
13	14.045	1858	1865	1870	rBV	239784	360333	6.91%	0.659%
14	14.592	1950	1958	1965	rVV	1160189	1933140	37.07%	3.537%
15	14.656	1965	1969	1975	rVB	45470	74183	1.42%	0.136%
16	14.997	2020	2027	2035	rVB	34896	73337	1.41%	0.134%
17	15.638	2131	2136	2141	rVB2	39777	64175	1.23%	0.117%
18	15.937	2183	2187	2193	rVB	30287	52691	1.01%	0.096%
19	16.078	2204	2211	2220	rBV	2430452	3760977	72.11%	6.881%
20	16.319	2247	2252	2255	rBV3	55357	75429	1.45%	0.138%
21	16.989	2362	2366	2374	rVB2	39728	72193	1.38%	0.132%
22	17.159	2391	2395	2404	rVB2	54771	107825	2.07%	0.197%
23	17.336	2419	2425	2429	rBV	1334665	2060479	39.51%	3.770%
24	17.377	2429	2432	2438	rVV	734991	1044664	20.03%	1.911%
25	17.465	2442	2447	2453	rVB	173719	283577	5.44%	0.519%
26	17.729	2488	2492	2497	rBV2	51601	83767	1.61%	0.153%
27	17.853	2509	2513	2519	rVB2	47907	70103	1.34%	0.128%
28	18.211	2570	2574	2578	rBV	106360	174042	3.34%	0.318%
29	18.258	2578	2582	2587	rVB	157863	243320	4.67%	0.445%
30	18.340	2592	2596	2601	rVV	57935	84954	1.63%	0.155%
31	18.405	2601	2607	2611	rVV2	160660	299097	5.73%	0.547%
32	18.440	2611	2613	2620	rVB	84685	111174	2.13%	0.203%
33	18.540	2626	2630	2637	rBV2	46864	73545	1.41%	0.135%
34	18.711	2655	2659	2662	rBV	88058	124373	2.38%	0.228%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

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_G\METHODS\8270-BG123019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.746	2662	2665	2670	rVB2	47574	71620	1.37%	0.131%
36	19.128	2726	2730	2734	rVB	69510	96602	1.85%	0.177%
37	19.169	2734	2737	2743	rBV4	79404	133320	2.56%	0.244%
38	19.263	2749	2753	2758	rBV2	67276	94244	1.81%	0.172%
39	19.386	2769	2774	2779	rVB	1335355	1846337	35.40%	3.378%
40	19.745	2826	2835	2844	rBV	1261017	2153166	41.29%	3.939%
41	19.821	2845	2848	2856	rVB2	62029	105720	2.03%	0.193%
42	19.950	2864	2870	2875	rBV	3946272	5215306	100.00%	9.542%
43	20.068	2887	2890	2896	rVB3	59315	130576	2.50%	0.239%
44	20.238	2916	2919	2922	rVV	111098	138198	2.65%	0.253%
45	20.273	2922	2925	2929	rVB	95496	110877	2.13%	0.203%
46	20.538	2967	2970	2973	rBV	66253	78570	1.51%	0.144%
47	20.761	3006	3008	3014	rBV2	75096	73192	1.40%	0.134%
48	20.990	3044	3047	3053	rVB	107792	167744	3.22%	0.307%
49	21.261	3088	3093	3099	rBV3	503242	825905	15.84%	1.511%
50	21.584	3141	3148	3153	rBV3	1392654	3079145	59.04%	5.633%
51	21.631	3153	3156	3166	rVB	442657	738957	14.17%	1.352%
52	23.728	3509	3513	3521	rBV2	240119	636174	12.20%	1.164%
53	24.721	3675	3682	3689	rBV3	672837	1774901	34.03%	3.247%

Sum of corrected areas: 54658760

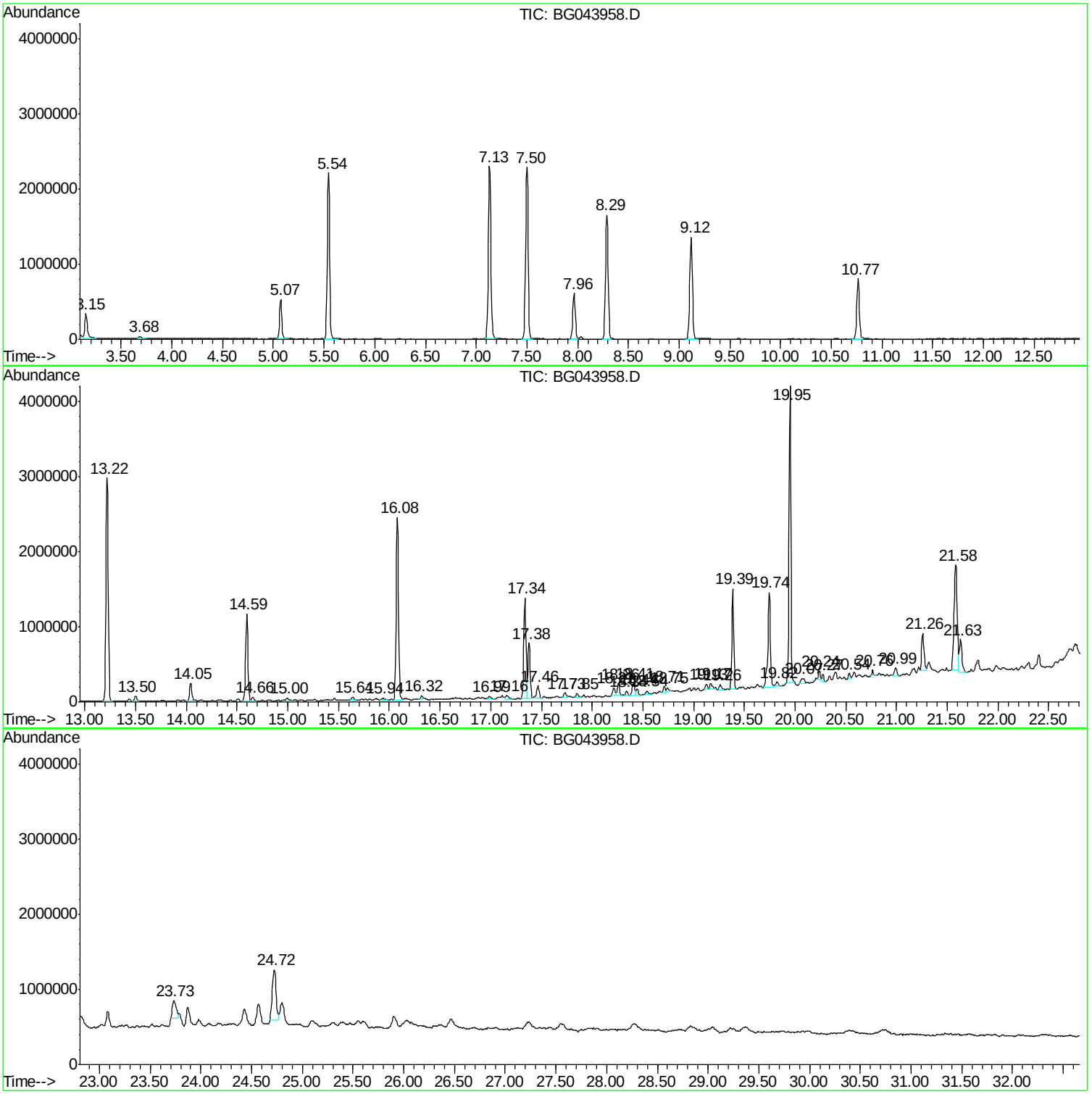
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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 G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

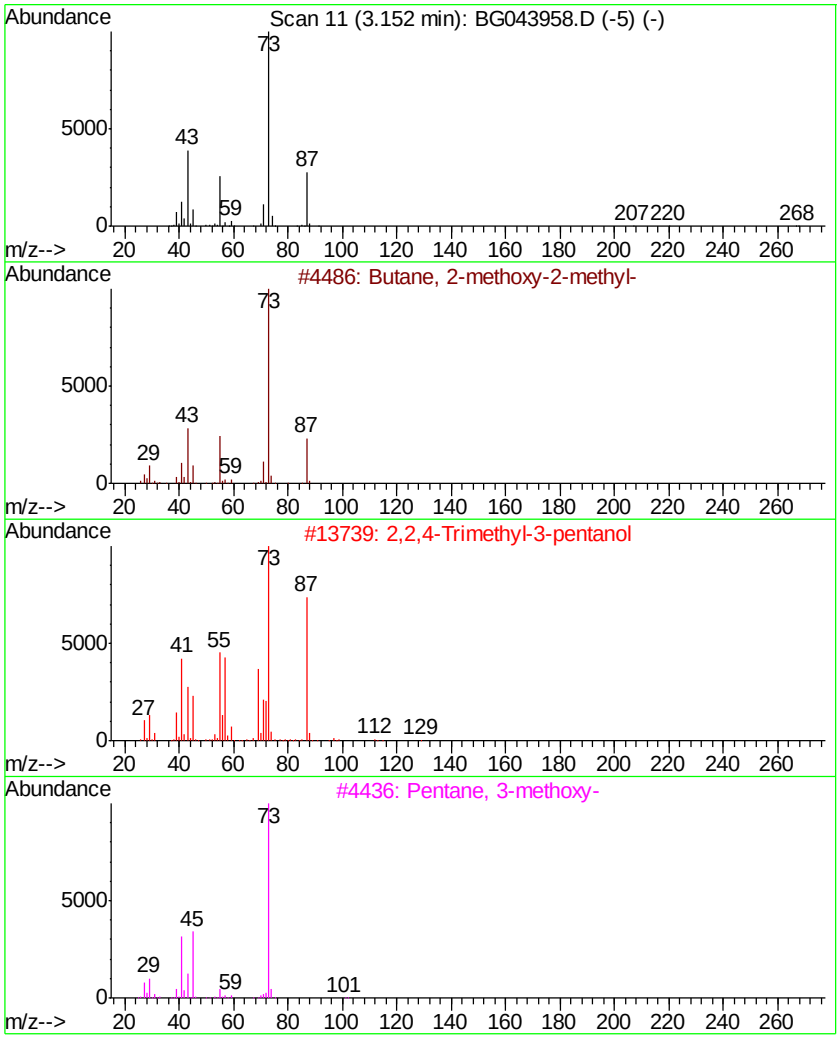
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

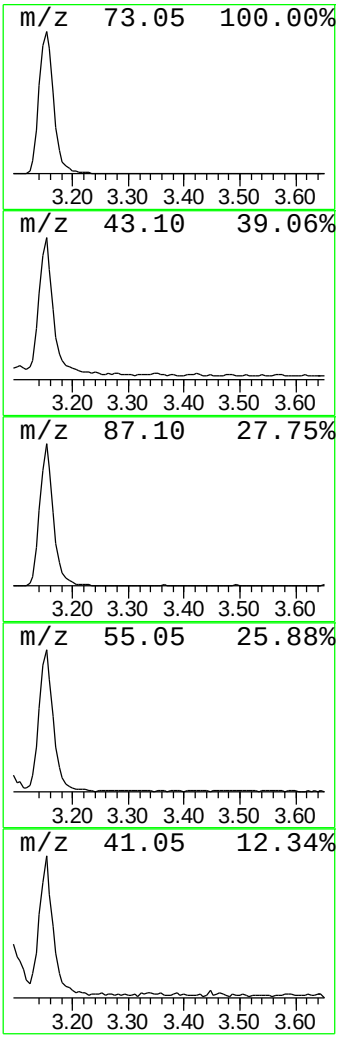
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	11.45 ng	590468	1,4-Dichlorobenzene-d4	7.96

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	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

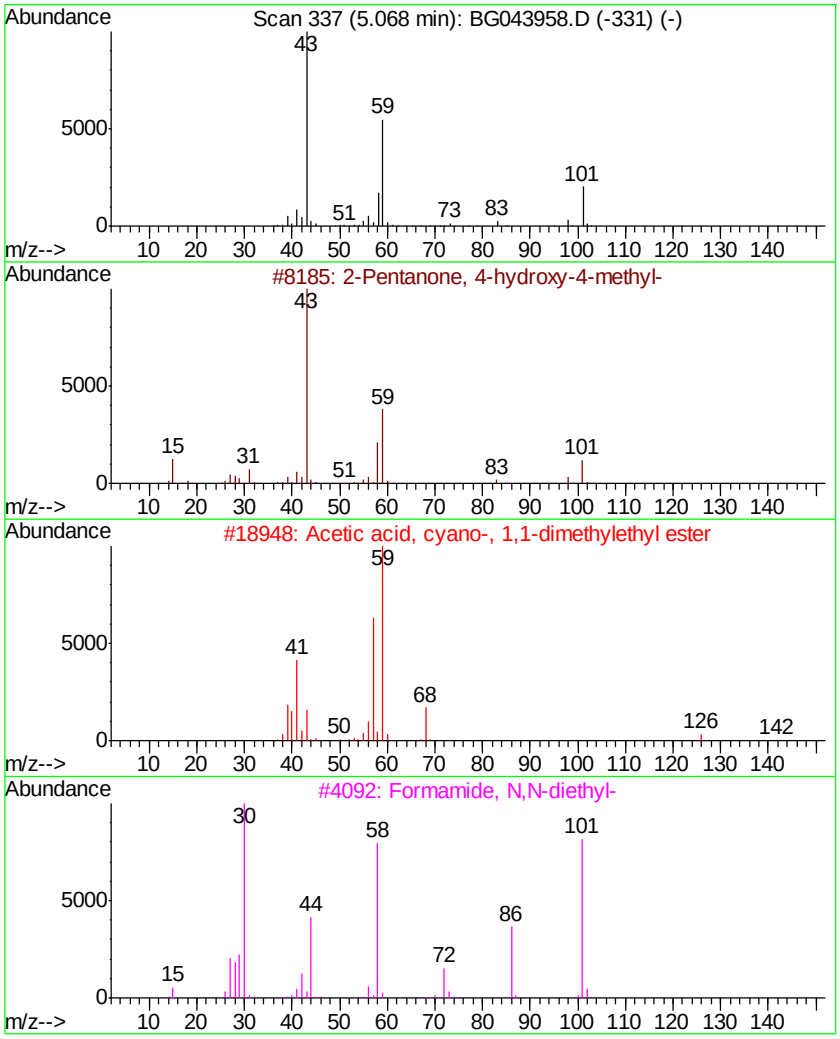
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

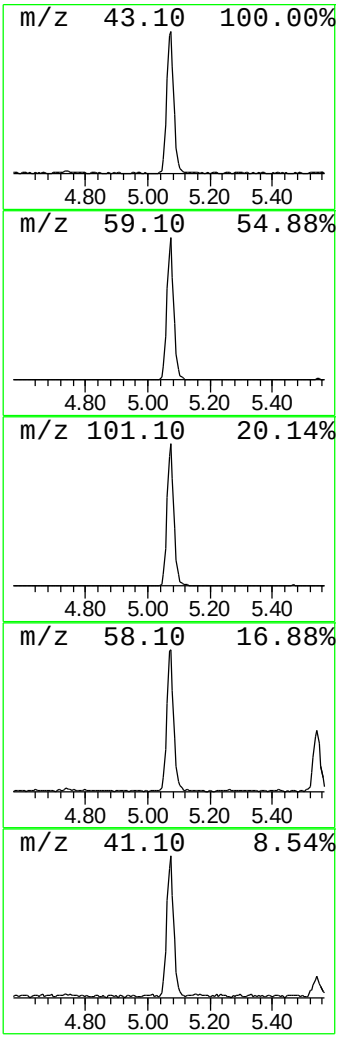
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	16.11 ng	830562	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

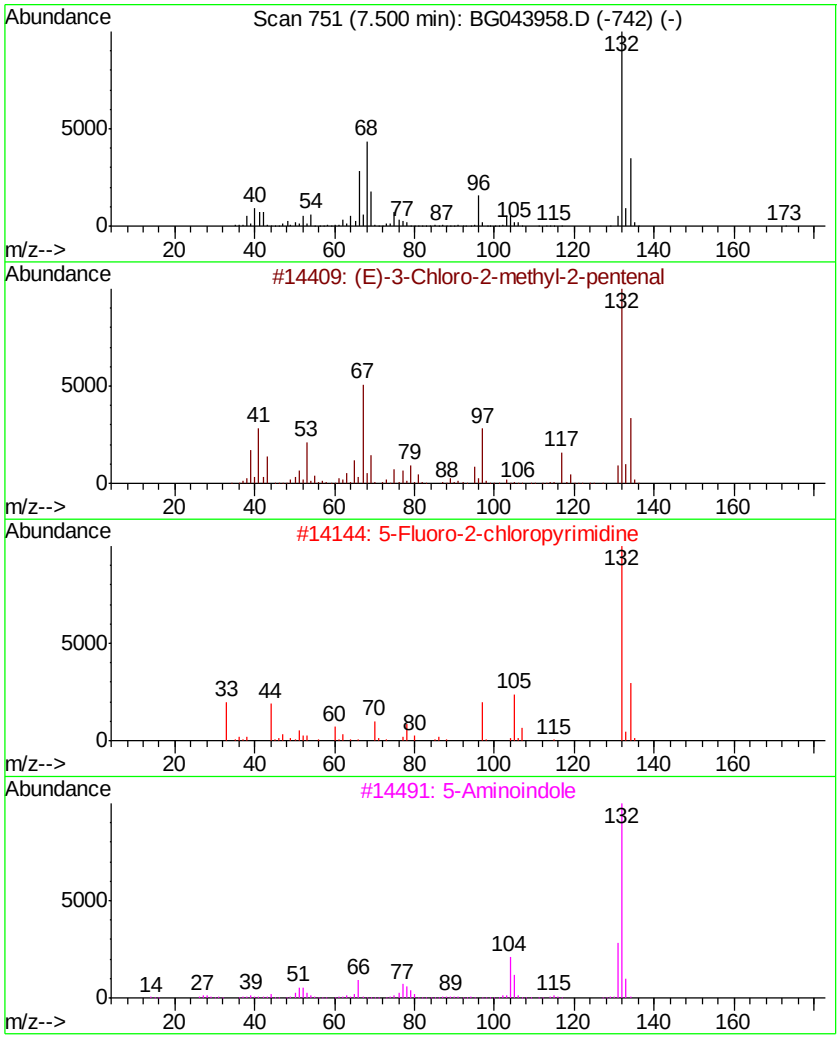
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

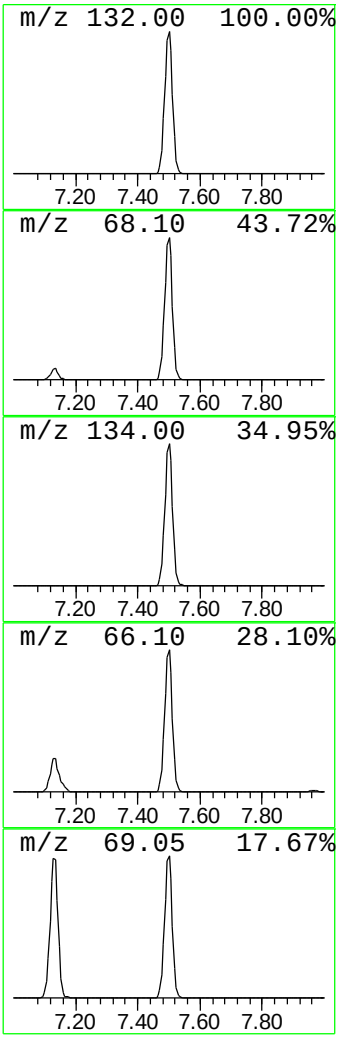
****

Peak Number 3 unknown7.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	78.15 ng	4029330	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

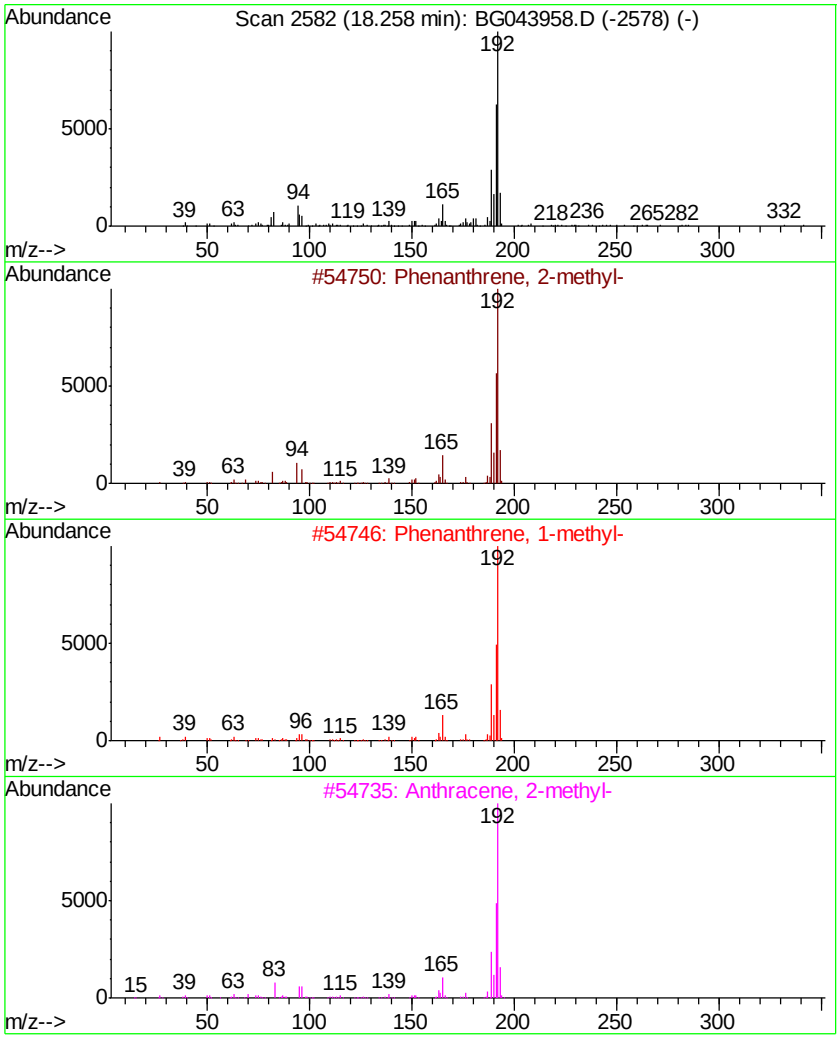
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

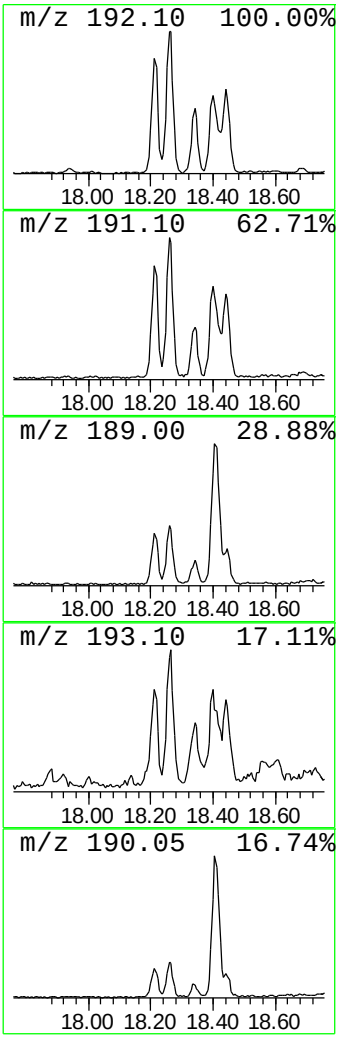
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.36 ng	243320	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

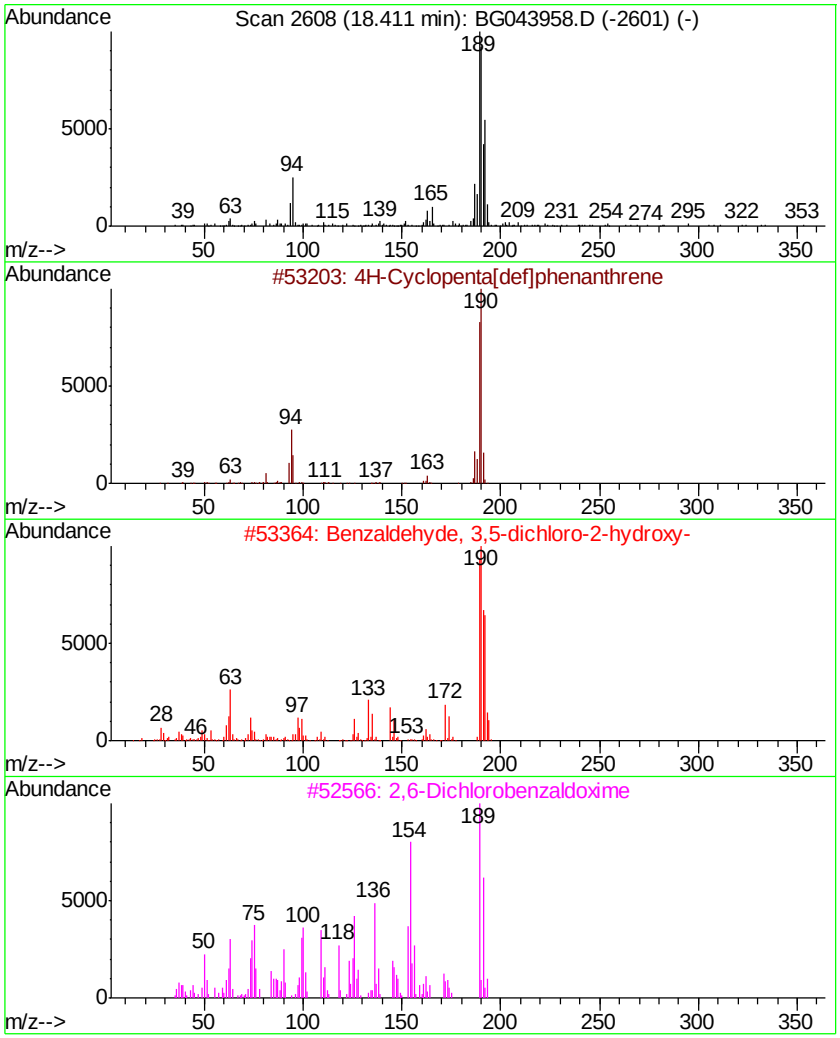
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

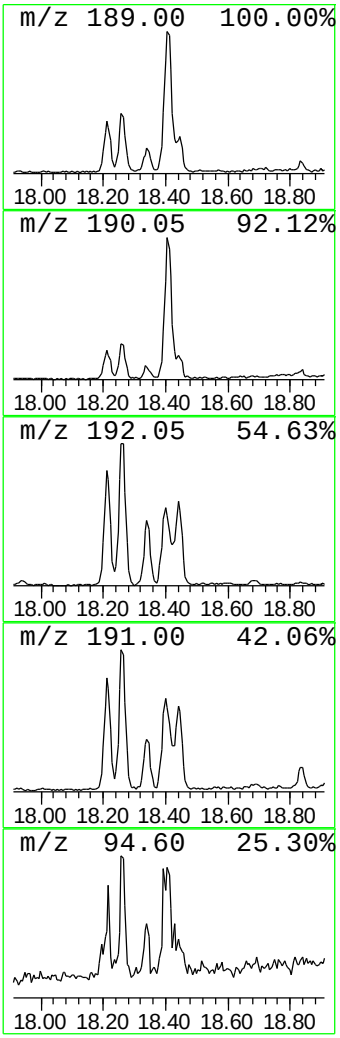
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	2.90 ng	299097	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	38
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
5	1-(3-Nitro-phenyl)-pyrrolidine	192	C10H12N2O2	1000300-34-7	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

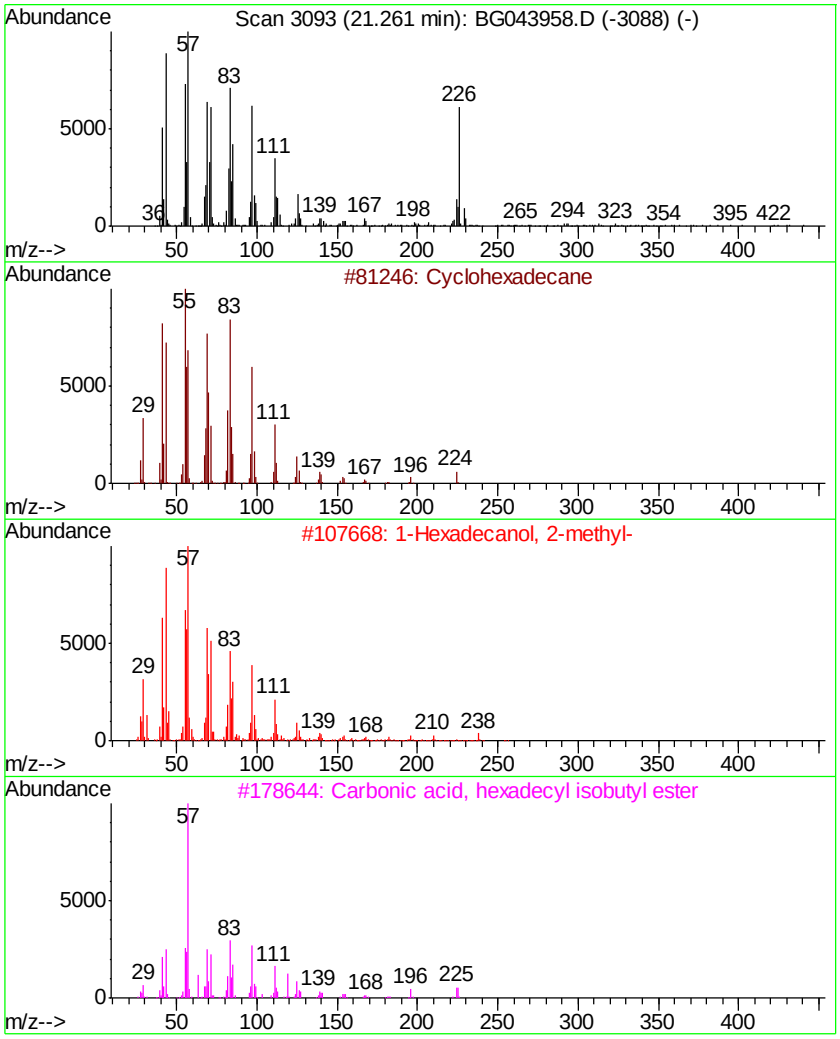
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

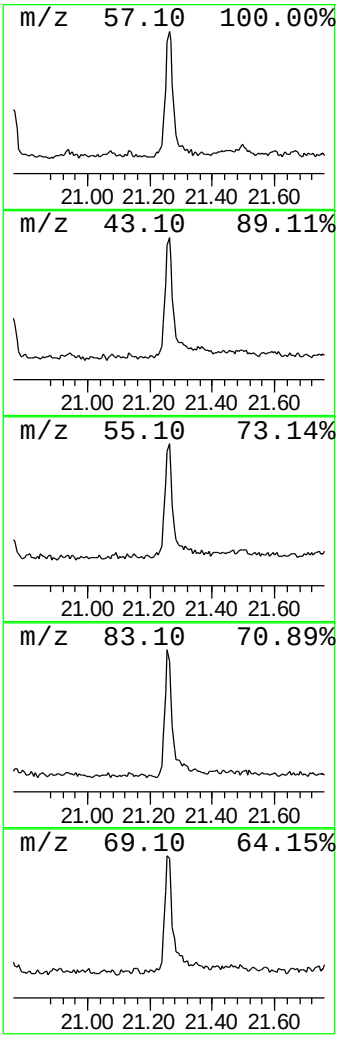
****

Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	5.36 ng	825905	Chrysene-d12	21.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	83
3	Carbonic acid, hexadecyl isobutyl...	342	C21H42O3	1000314-61-3	81
4	Trihexadecyl borate	735	C48H99BO3	002665-11-4	81
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG010720\
Data File : BG043958.D
Acq On : 7 Jan 2020 17:35
Operator : JU
Sample : K6463-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-6-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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...	3.15	11.4	ng	590468	1	7.96	1031210	20.0
2-Pentanone, 4-hy...	5.07	16.1	ng	830562	1	7.96	1031210	20.0
unknown7.50	7.50	78.2	ng	4029330	1	7.96	1031210	20.0
Phenanthrene, 2-m...	18.26	2.4	ng	243320	4	17.34	2060480	20.0
4H-Cyclopenta[def...	18.41	2.9	ng	299097	4	17.34	2060480	20.0
Cyclohexadecane	21.26	5.4	ng	825905	5	21.59	3079150	20.0