LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

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-BG102119.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	3.190	11	17	31	rVB	85854	219600	11.26%	1.917%
2	4.524	238	244	252	rBV	38091	68822	3.53%	0.601%
3	5.123	336	346	359	rBV	470534	813080	41.71%	7.098%
4	5.605	422	428	440	rBV	95702	191052	9.80%	1.668%
5	6.698	610	614	619	rVB2	19845	33684	1.73%	0.294%
6	7.203	689	700	714	rBV	424859	879803	45.13%	7.680%
7	7.555	753	760	771	rBV	324522	580549	29.78%	5.068%
8	8.014	830	838	846	rBV	181166	322738	16.56%	2.817%
9	8.337	881	893	903	rBV	462176	835243	42.84%	7.291%
10	9.177	1023	1036	1045	rBV	299247	611496	31.37%	5.338%
11	10.816	1305	1315	1324	rBV	205535	419146	21.50%	3.659%
12	13.172	1711	1716	1723	rVB5	12016	22875	1.17%	0.200%
13	13.260	1723	1731	1742	rBV	863348	1442288	73.98%	12.590%
14	13.966	1846	1851	1856	rBV7	31223	52272	2.68%	0.456%
15	14.089	1863	1872	1881	rBV	81571	164355	8.43%	1.435%
16	14.389	1912	1923	1925	rBV8	13014	34364	1.76%	0.300%
17	14.471	1932	1937	1942	rVB4	23297	39758	2.04%	0.347%
18	14.535	1943	1948	1952	rVB4	13801	22017	1.13%	0.192%
19	14.600	1954	1959	1961	rBV2	61446	90893	4.66%	0.793%
20	14.641	1961	1966	1974	rVB	340932	546904	28.05%	4.774%
21	14.888	2004	2008	2013	rVB4	38436	51815	2.66%	0.452%
22	15.429	2094	2100	2105	rBV9	15311	28818	1.48%	0.252%
23	15.481	2105	2109	2112	rVB3	17329	21643	1.11%	0.189%
24	15.887	2175	2178	2183	rVB4	12594	21366	1.10%	0.187%
25	16.134	2216	2220	2229	rVV2	35901	64481	3.31%	0.563%
26	16.204	2229	2232	2239	rVB7	12221	23384	1.20%	0.204%
27	16.363	2252	2259	2265	rBV5	34845	78338	4.02%	0.684%
28	17.179	2396	2398	2405	rVB7	12085	22503	1.15%	0.196%
29	17.385	2427	2433	2439	rBV	379705	631981	32.42%	5.517%
30	17.873	2513	2516	2519	rBV3	18822	24622	1.26%	0.215%
31	18.278	2581	2585	2590	rBV7	19865	36674	1.88%	0.320%
32	18.560	2630	2633	2636	rBV3	22071	28384	1.46%	0.248%
33	19.189	2733	2740	2743	rBV5	31122	68167	3.50%	0.595%
34	19.441	2780	2783	2789	rBV	21871	29830	1.53%	0.260%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

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-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.994	2872	2877	2887	rVB	1405834	1949477	100.00%	17.017%
36	20.246	2917	2920	2924	rBV6	38975	66364	3.40%	0.579%
37	21.292	3094	3098	3109	rBV	130487	229739	11.78%	2.005%
38	21.657	3155	3160	3167	rVB	400843	687224	35.25%	5.999%

Sum of corrected areas: 11455749

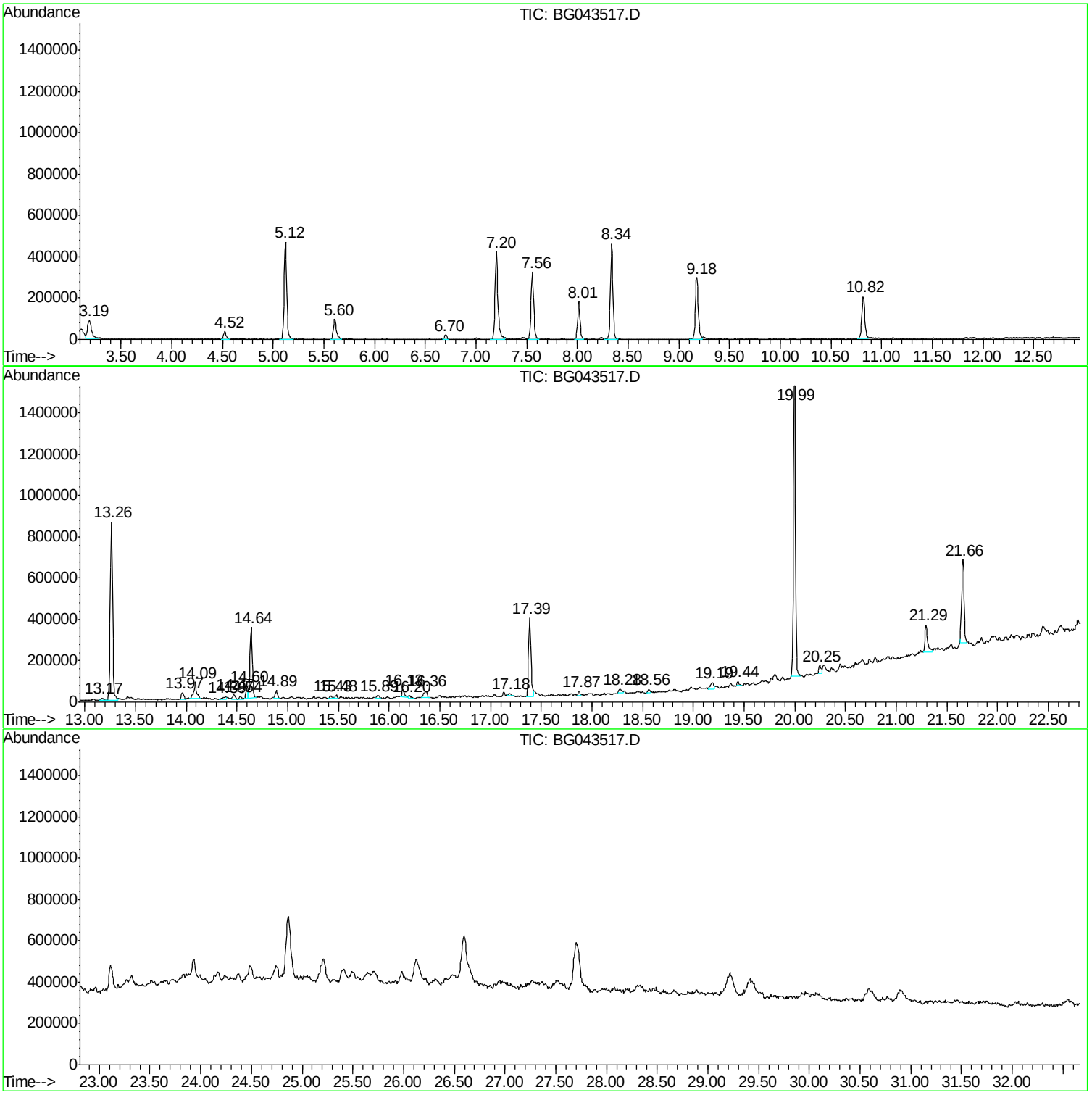
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

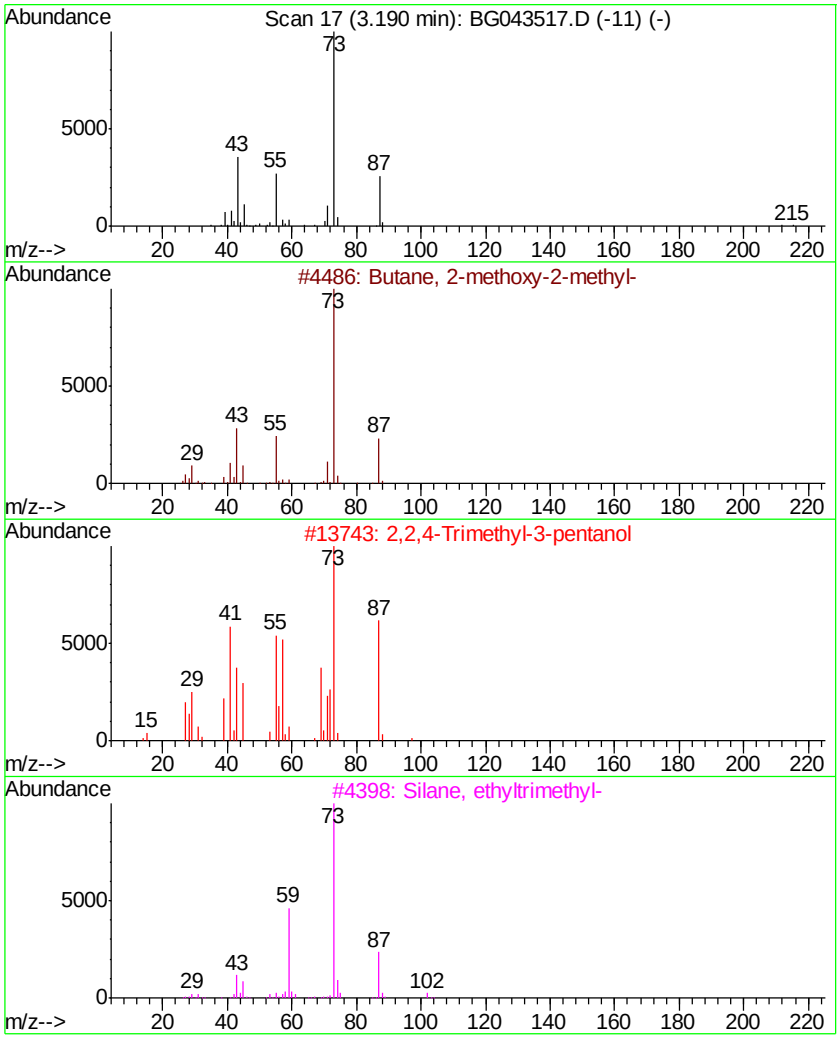
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

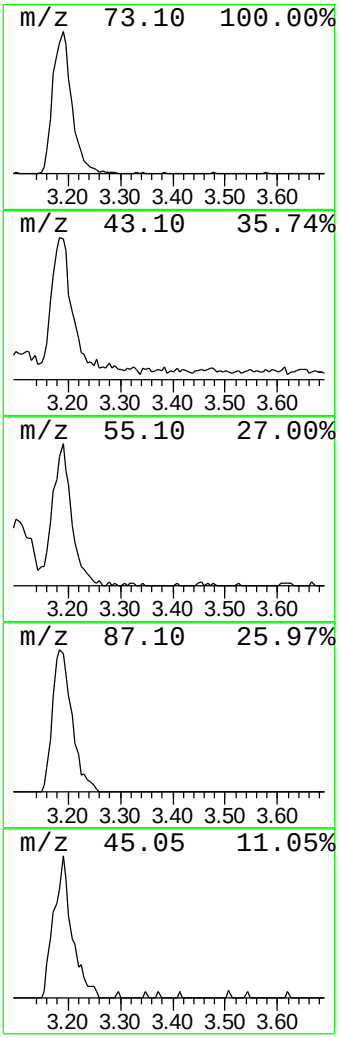
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	13.61 ng	219600	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

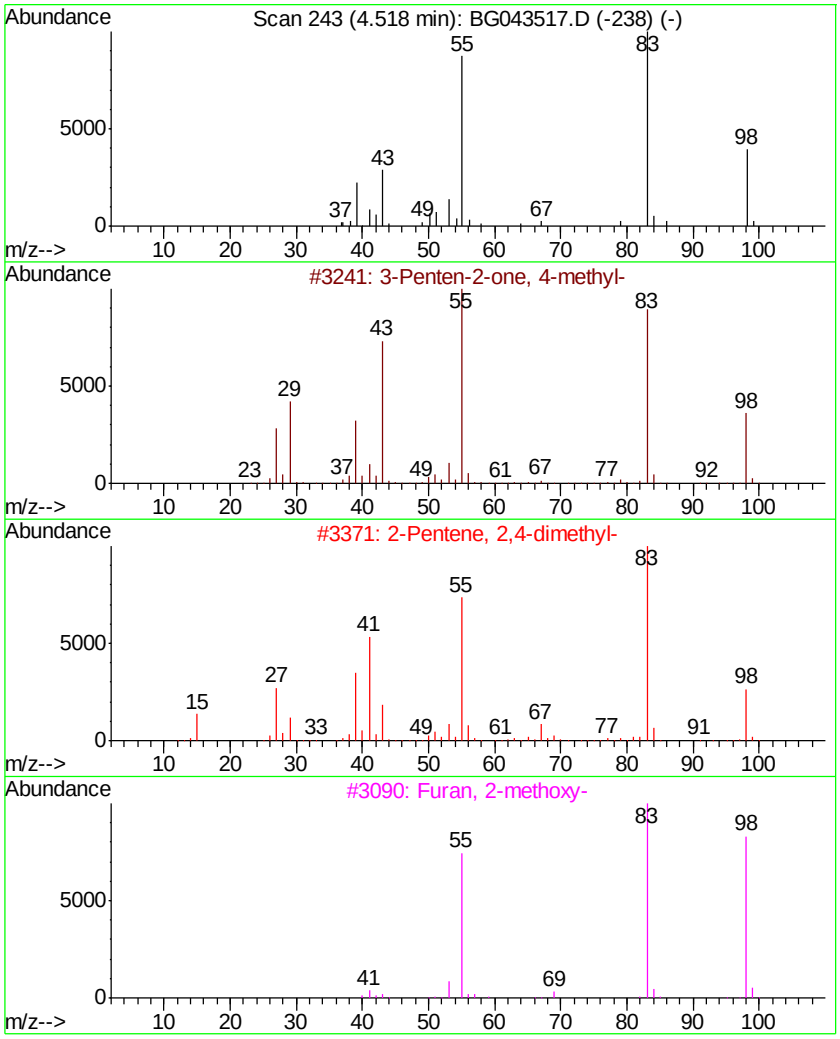
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

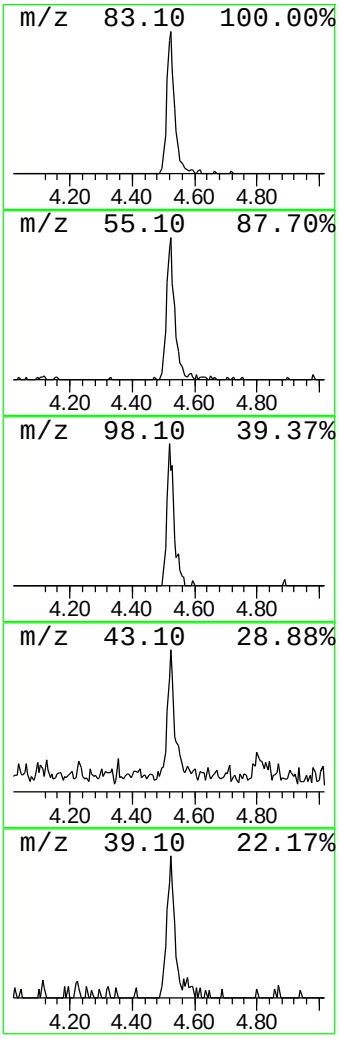
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	4.26 ng	68822	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
3	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	78
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

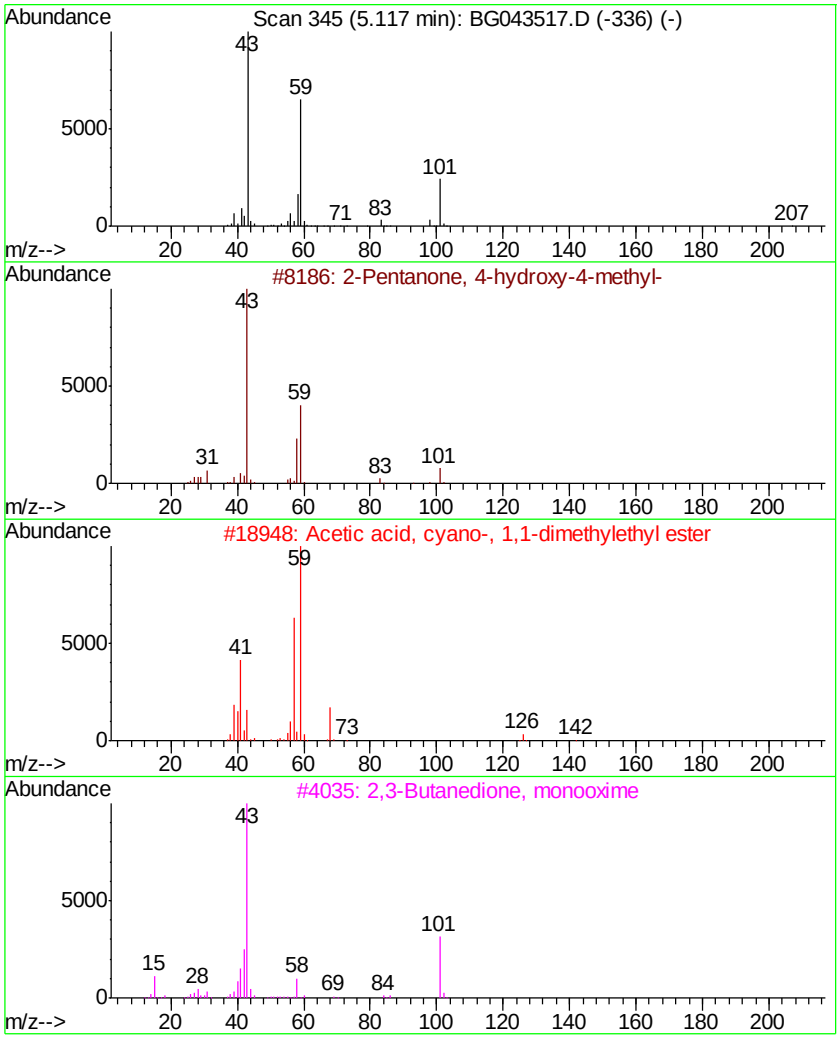
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

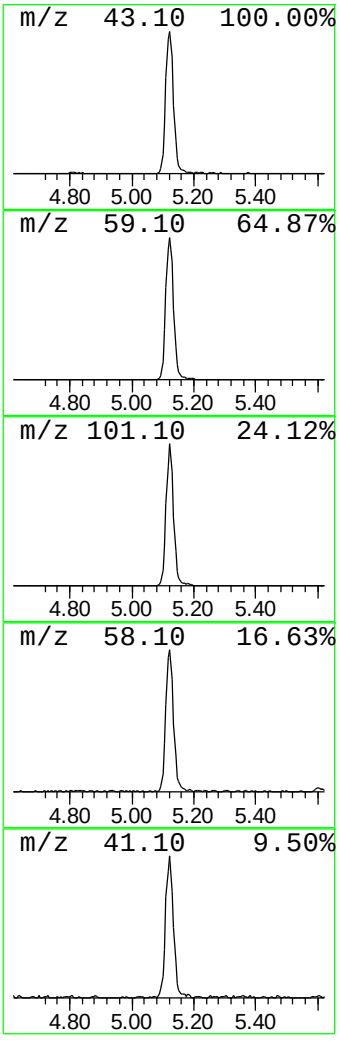
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	50.39 ng	813080	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

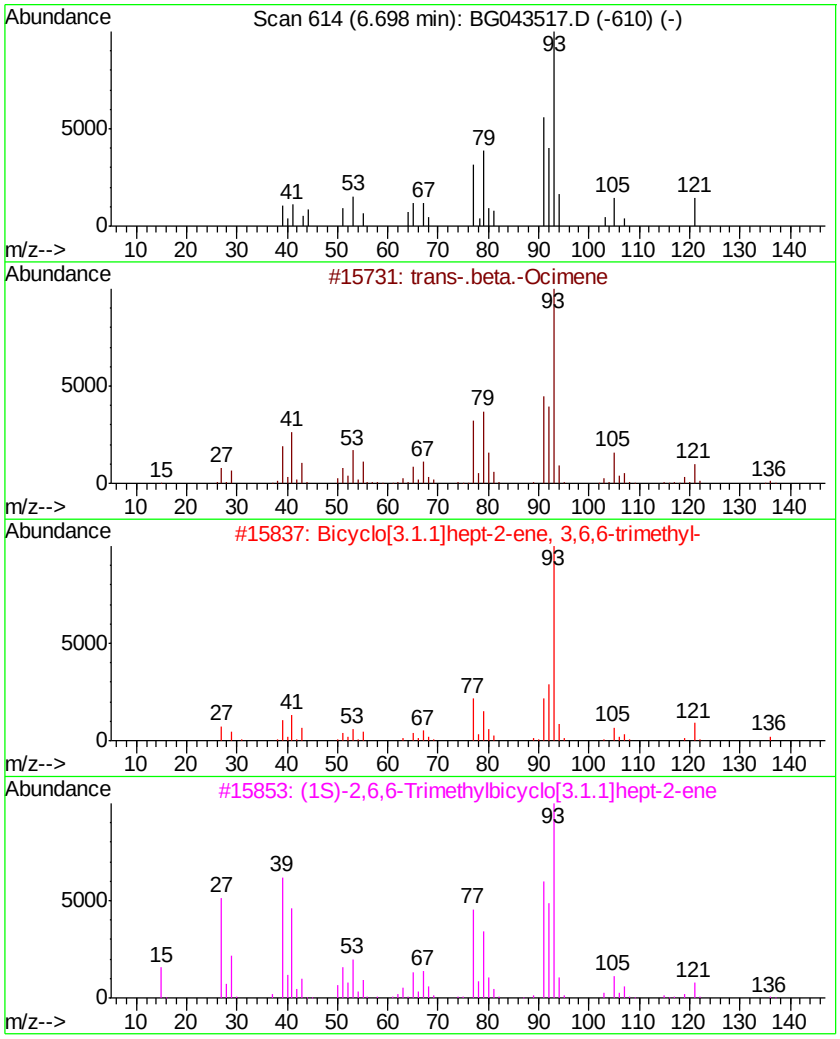
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

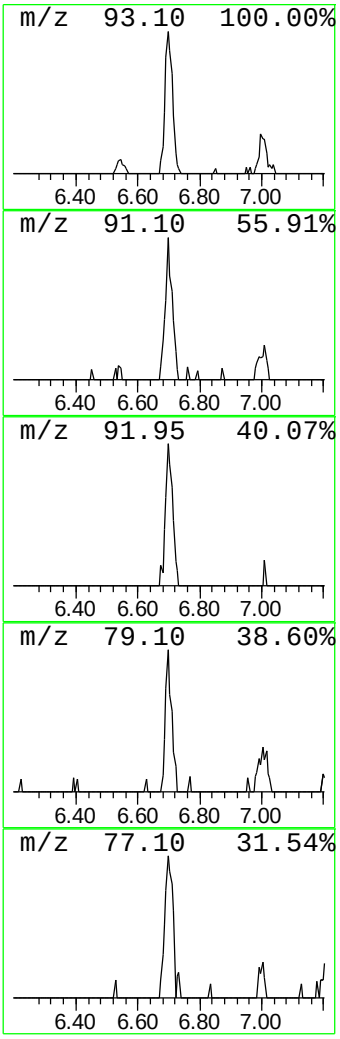
****

Peak Number 4 trans-.beta.-Ocimene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	2.09 ng	33684	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-.beta.-Ocimene	136	C10H16	003779-61-1	64
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	64
3	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	56
4	3,5-Methanocyclopentapyrazole, 3...	164	C10H16N2	087143-58-6	37
5	9,10-Epoxy-4,8-ethanocyclohepta[...	208	C11H12O4	1000141-73-2	32





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

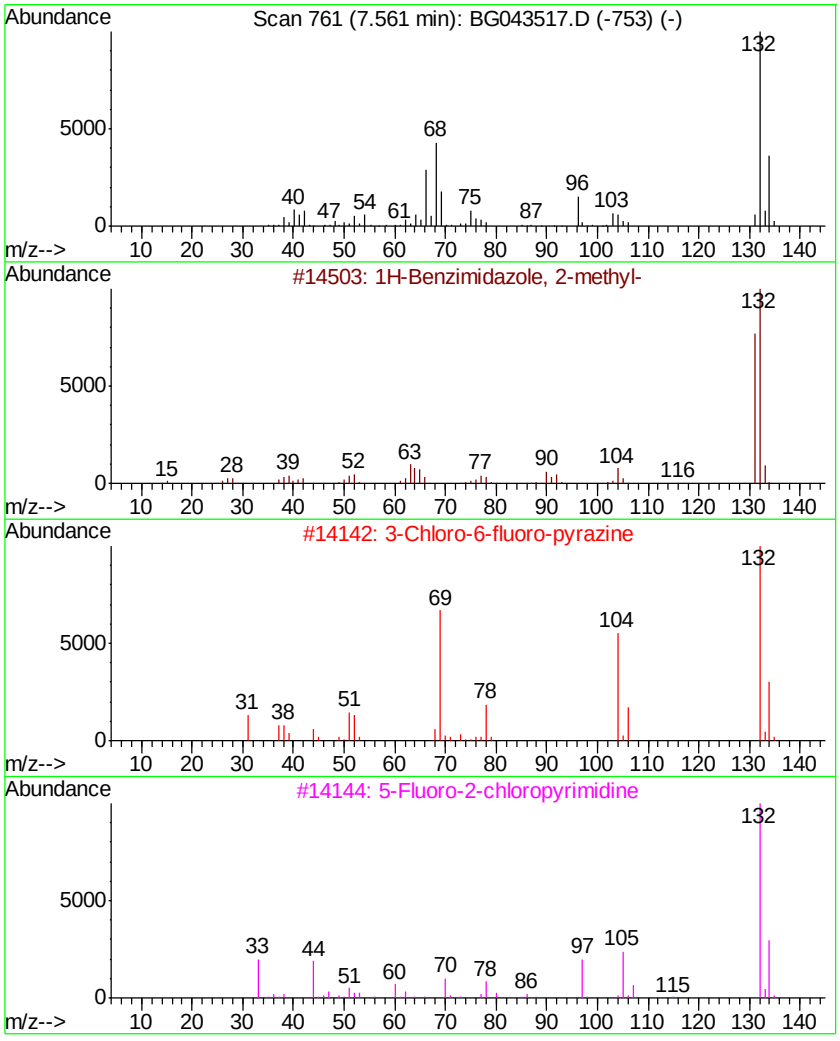
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

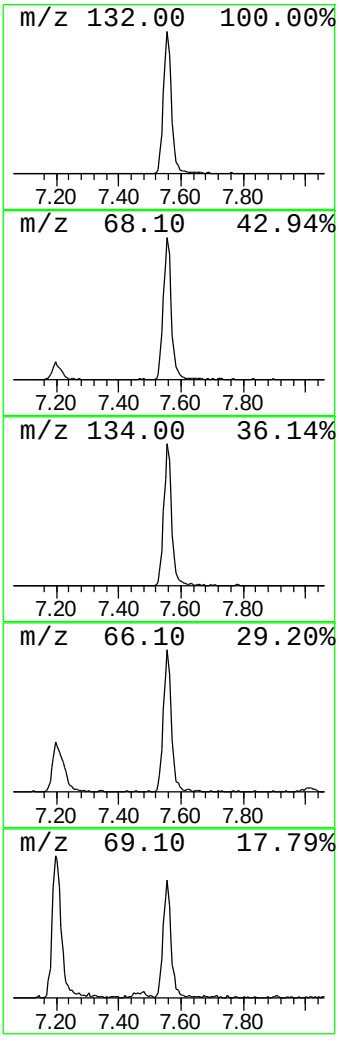
****

Peak Number 5 unknown7.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	35.98 ng	580549	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

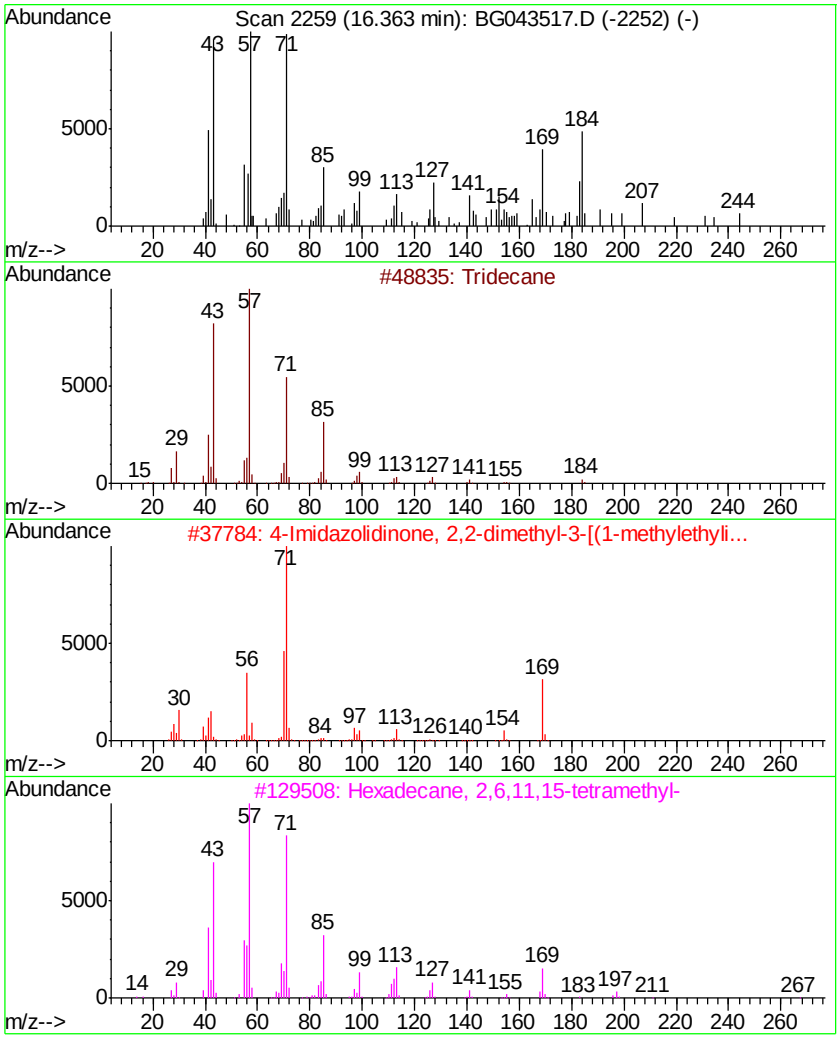
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

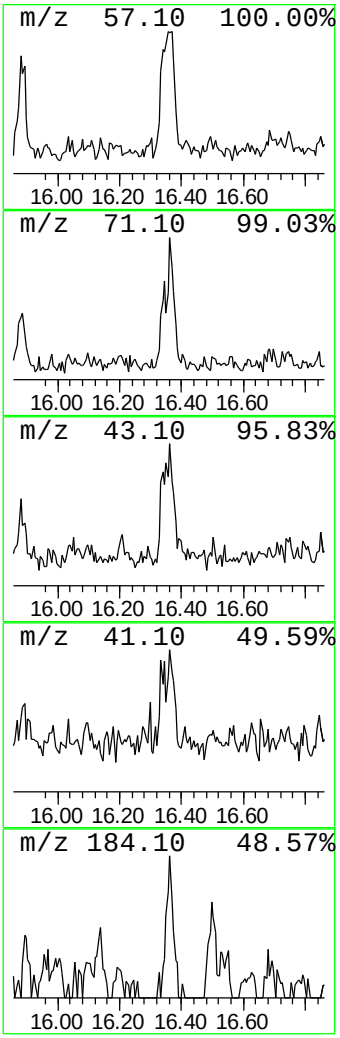
****

Peak Number 7 unknown16.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.48 ng	78338	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	49
2	4-Imidazolidinone, 2,2-dimethyl-...	169	C8H15N3O	142071-78-1	38
3	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	35
4	Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	35
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

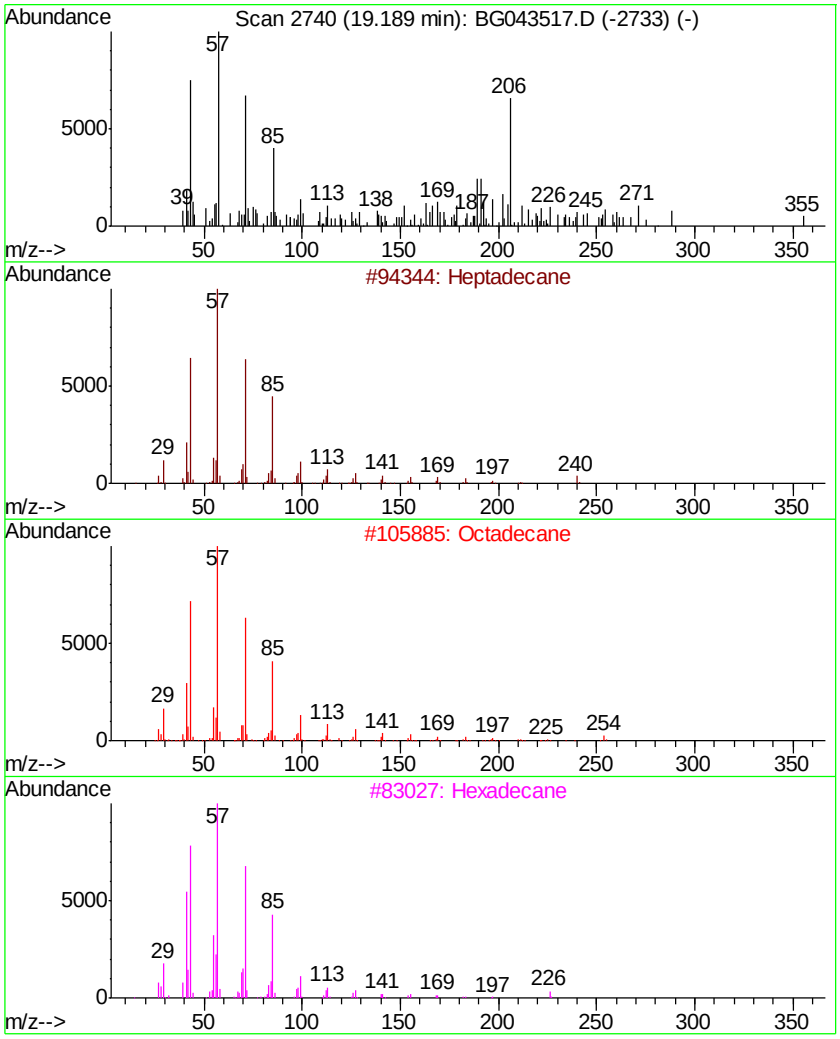
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

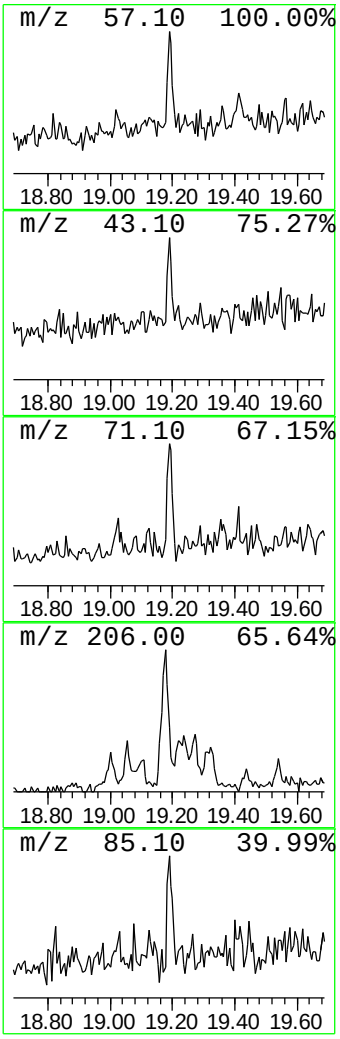
****

Peak Number 8 unknown19.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	2.16 ng	68167	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	42
2	Octadecane	254	C18H38	000593-45-3	42
3	Hexadecane	226	C16H34	000544-76-3	42
4	Tridecane	184	C13H28	000629-50-5	42
5	Dodecane	170	C12H26	000112-40-3	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

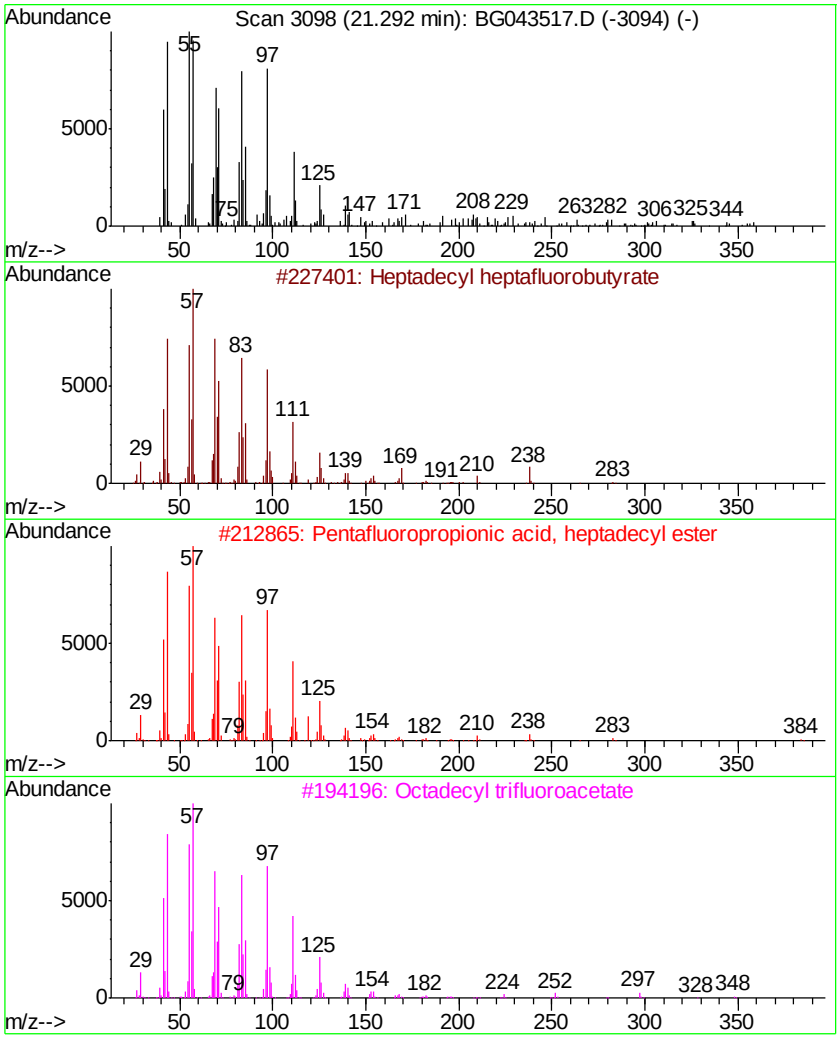
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

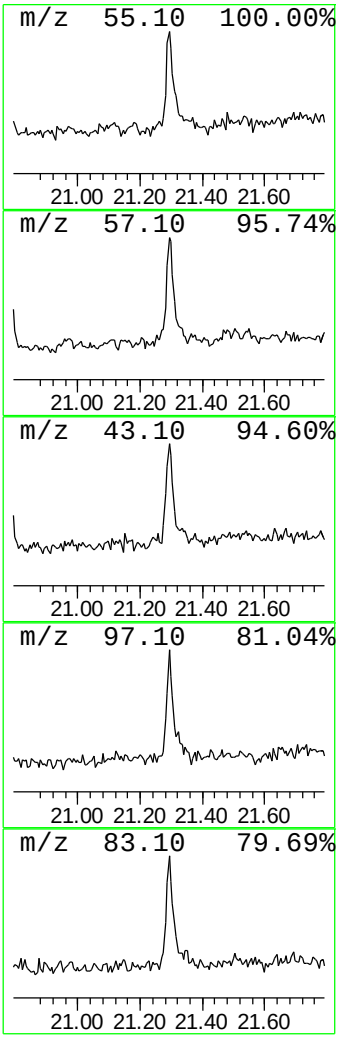
****

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	6.69 ng	229739	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110519\
Data File : BG043517.D
Acq On : 5 Nov 2019 21:03
Operator : JU
Sample : K5662-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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...	3.19	13.6	ng	219600	1	8.01	322738	20.0
3-Penten-2-one, 4...	4.52	4.3	ng	68822	1	8.01	322738	20.0
2-Pentanone, 4-hy...	5.12	50.4	ng	813080	1	8.01	322738	20.0
trans-.beta.-Ocimene	6.70	2.1	ng	33684	1	8.01	322738	20.0
unknown7.56	7.56	36.0	ng	580549	1	8.01	322738	20.0
unknown16.36	16.36	2.5	ng	78338	4	17.39	631981	20.0
unknown19.19	19.19	2.2	ng	68167	4	17.39	631981	20.0
Heptadecyl heptaf...	21.29	6.7	ng	229739	5	21.66	687224	20.0