LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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	3.194	13	18	27	rVB	111930	173384	8.58%	1.082%
2	5.127	342	347	357	rBV	91214	154236	7.63%	0.963%
3	5.614	423	430	443	rBV	458004	831857	41.15%	5.193%
4	7.212	694	702	719	rBV	496794	985830	48.77%	6.154%
5	7.565	755	762	773	rBV	523930	956021	47.30%	5.968%
6	8.023	833	840	849	rBV	151919	268193	13.27%	1.674%
7	8.346	887	895	905	rBV	397286	700059	34.63%	4.370%
8	9.187	1029	1038	1052	rBV	269569	560743	27.74%	3.500%
9	10.832	1310	1318	1334	rBV	169913	374455	18.52%	2.338%
10	13.276	1725	1734	1750	rBV	758682	1298011	64.21%	8.103%
11	14.104	1869	1875	1890	rBV	73993	144595	7.15%	0.903%
12	14.651	1961	1968	1975	rBV2	344015	560324	27.72%	3.498%
13	14.715	1975	1979	1985	rVB	22146	37151	1.84%	0.232%
14	15.702	2142	2147	2154	rBV2	14846	27598	1.37%	0.172%
15	16.143	2214	2222	2239	rBV	692715	1274045	63.03%	7.953%
16	17.395	2429	2435	2439	rBV2	421300	670790	33.18%	4.187%
17	17.436	2439	2442	2450	rVV	221551	346069	17.12%	2.160%
18	17.524	2450	2457	2469	rVB3	44496	111539	5.52%	0.696%
19	17.818	2499	2507	2515	rBV4	11194	30491	1.51%	0.190%
20	18.282	2580	2586	2591	rBV5	48515	86647	4.29%	0.541%
21	18.470	2613	2618	2622	rBV2	27803	46603	2.31%	0.291%
22	19.445	2778	2784	2793	rBV	289654	448542	22.19%	2.800%
23	19.804	2834	2845	2853	rBV	258029	464574	22.98%	2.900%
24	20.003	2873	2879	2893	rBV	1481061	2021369	100.00%	12.618%
25	20.297	2920	2929	2935	rVB2	37950	69706	3.45%	0.435%
26	20.397	2941	2946	2952	rBV2	28837	43868	2.17%	0.274%
27	21.243	3085	3090	3094	rBV2	15901	27220	1.35%	0.170%
28	21.308	3094	3101	3104	rBV6	60589	130310	6.45%	0.813%
29	21.660	3151	3161	3166	rBV2	508678	1051432	52.02%	6.564%
30	21.707	3166	3169	3181	rVB2	101514	180402	8.92%	1.126%
31	21.848	3188	3193	3202	rBV4	45293	85241	4.22%	0.532%
32	22.447	3289	3295	3300	rBV3	47932	77664	3.84%	0.485%
33	23.135	3406	3412	3418	rVB3	50341	98630	4.88%	0.616%
34	23.329	3441	3445	3451	rVB4	18992	32763	1.62%	0.205%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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	23.846	3526	3533	3540	rBV3	64697	206766	10.23%	1.291%
36	24.098	3570	3576	3587	rVB2	14696	44131	2.18%	0.275%
37	24.557	3646	3654	3663	rBV	39783	107205	5.30%	0.669%
38	24.698	3670	3678	3692	rBV3	58439	179714	8.89%	1.122%
39	24.862	3694	3706	3714	rBV2	324307	977516	48.36%	6.102%
40	25.985	3890	3897	3904	rVB4	28037	64917	3.21%	0.405%
41	28.476	4313	4321	4322	rBV4	19999	38956	1.93%	0.243%
42	29.610	4507	4514	4515	rBV4	16863	29575	1.46%	0.185%

Sum of corrected areas: 16019142

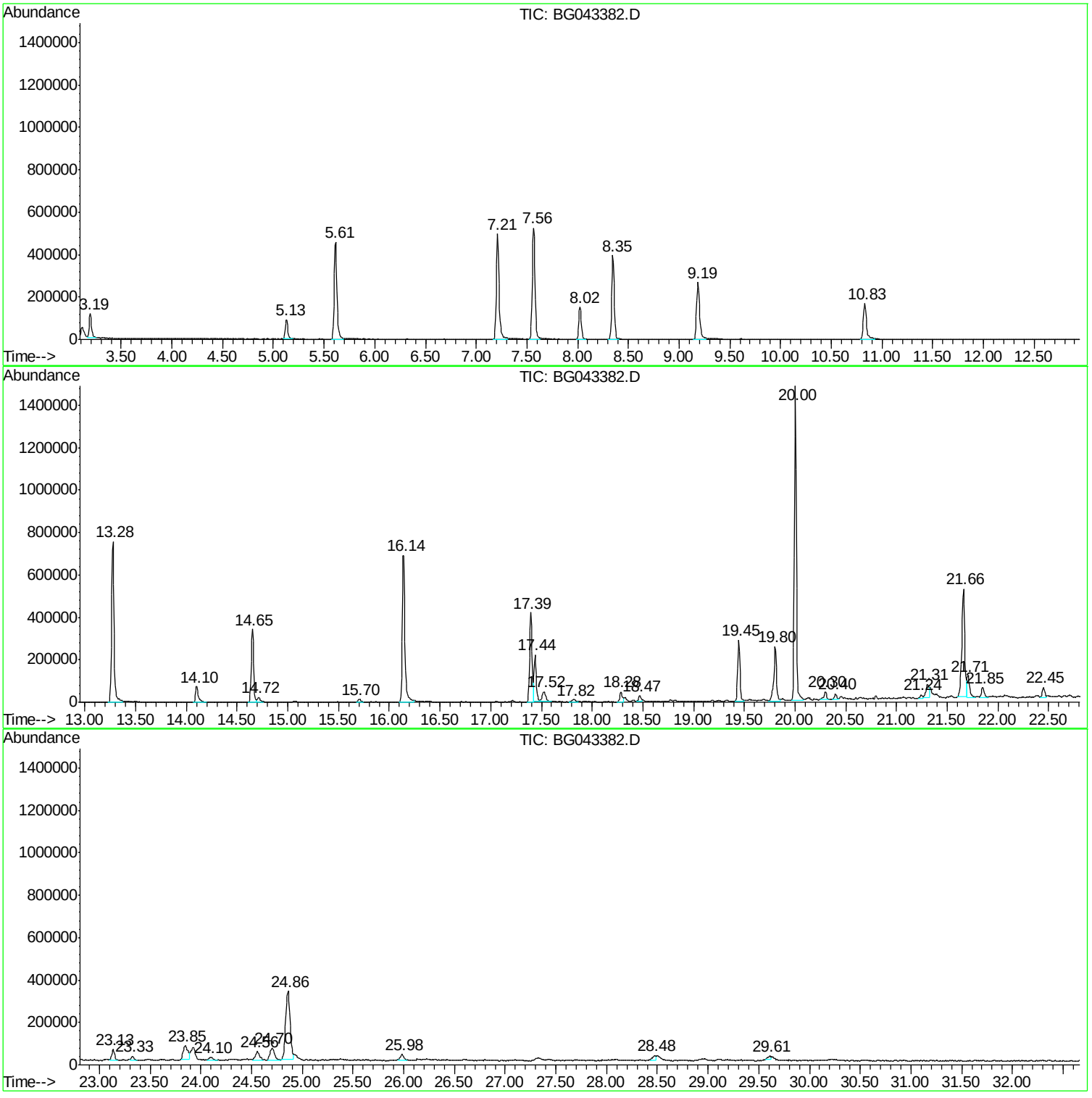
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-20-(0-2.5)

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\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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

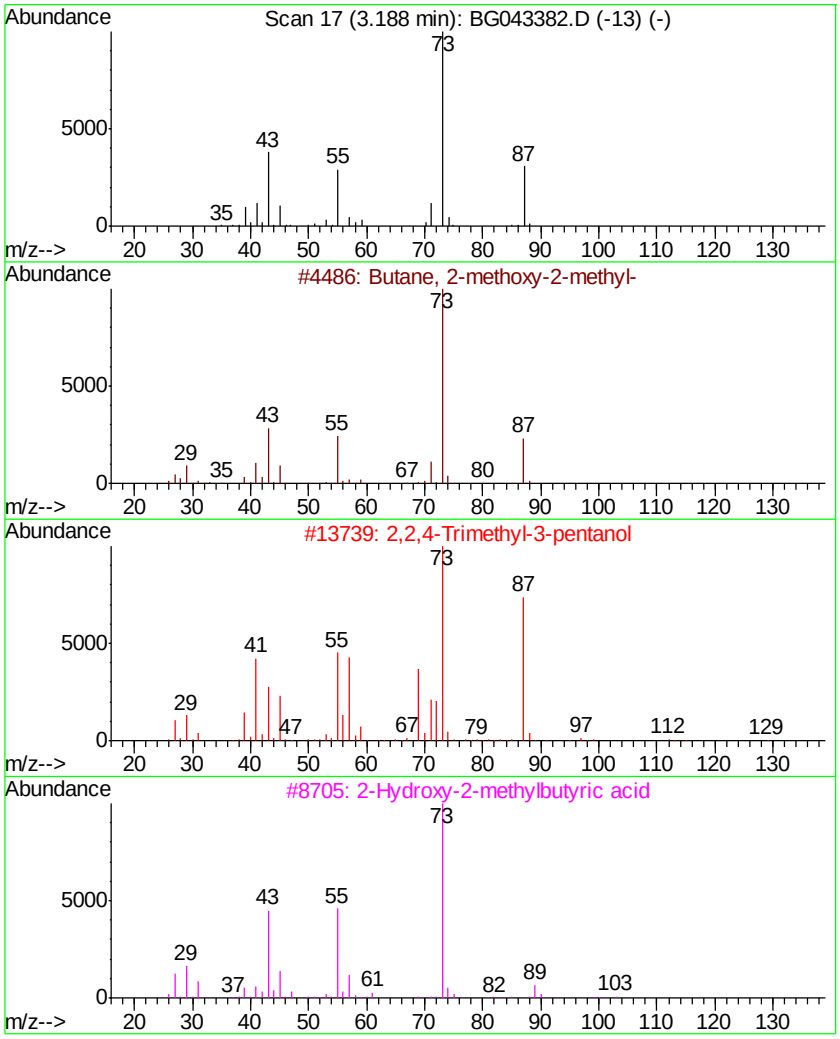
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

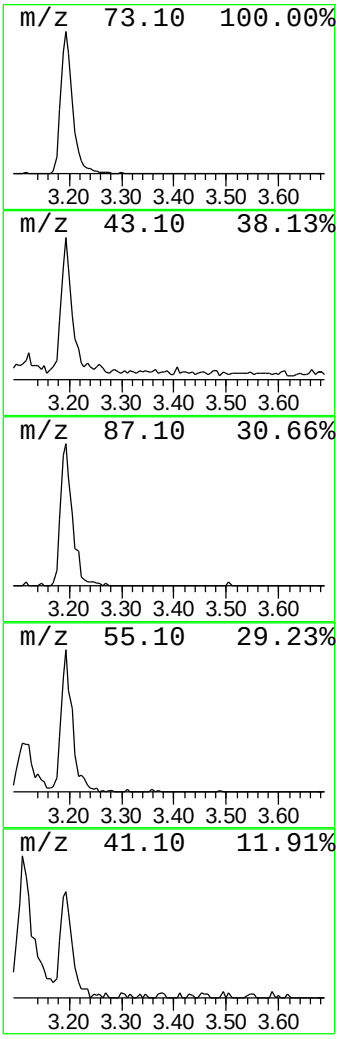
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	12.93 ng	173384	1,4-Dichlorobenzene-d4	8.02

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	40
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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

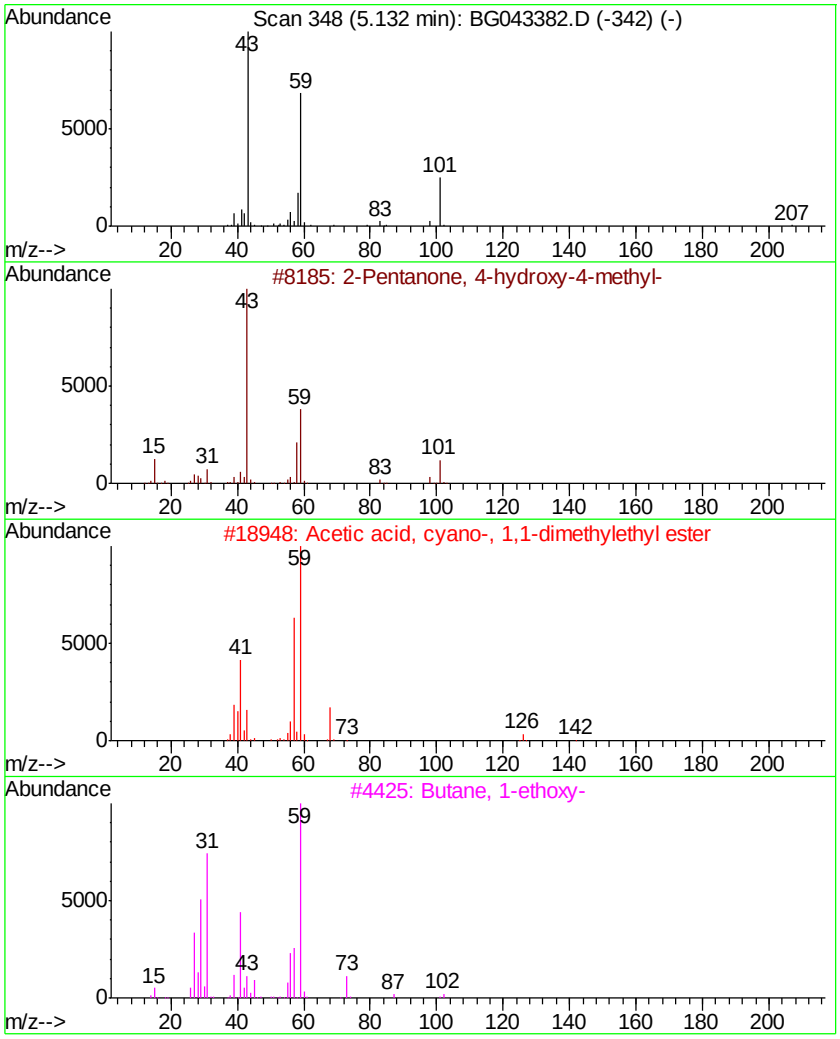
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

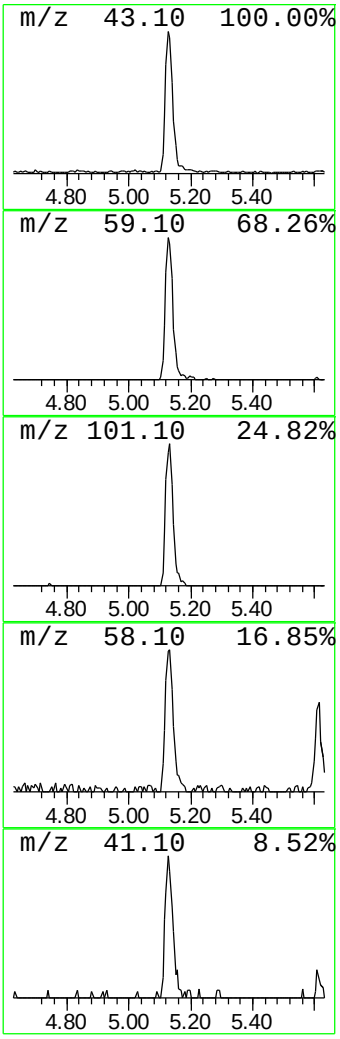
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	11.50 ng	154236	1,4-Dichlorobenzene-d4	8.02

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	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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

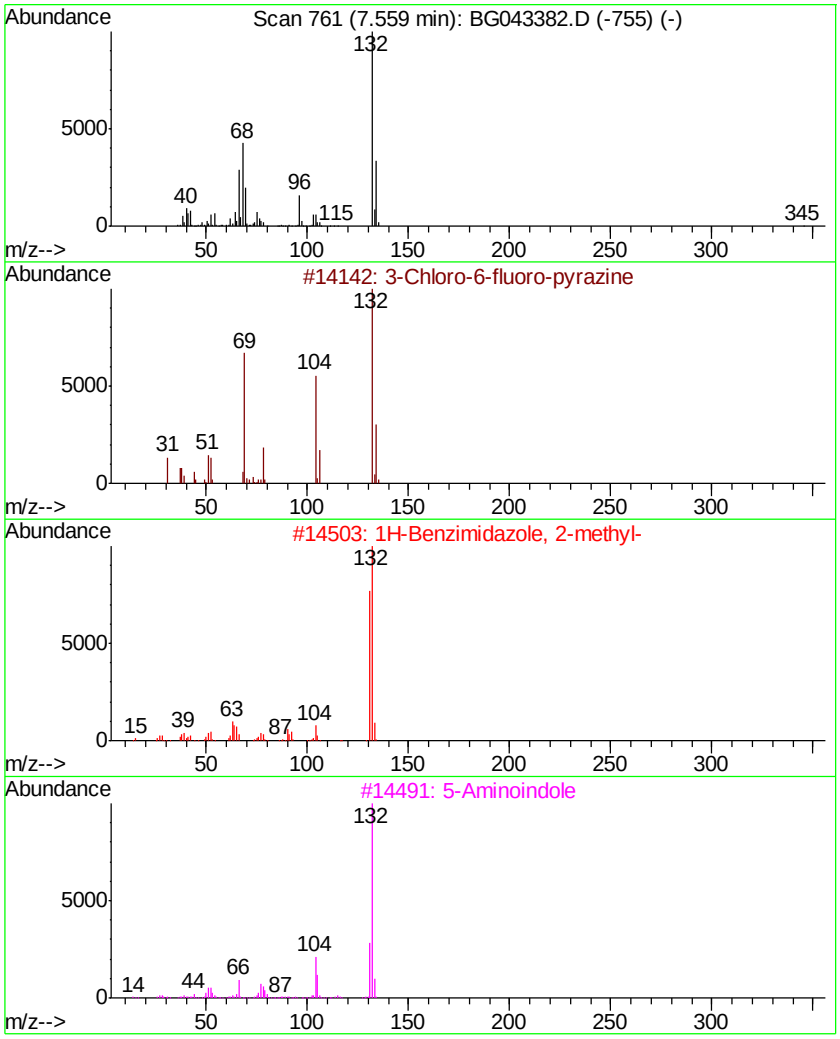
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

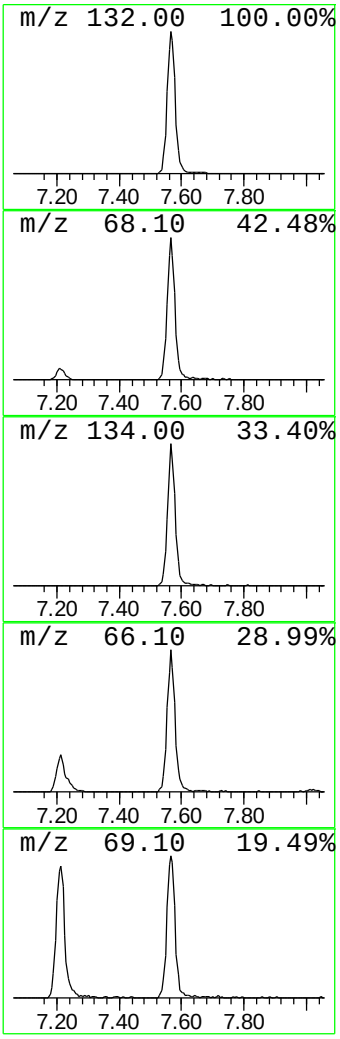
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	71.29 ng	956021	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	16
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





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Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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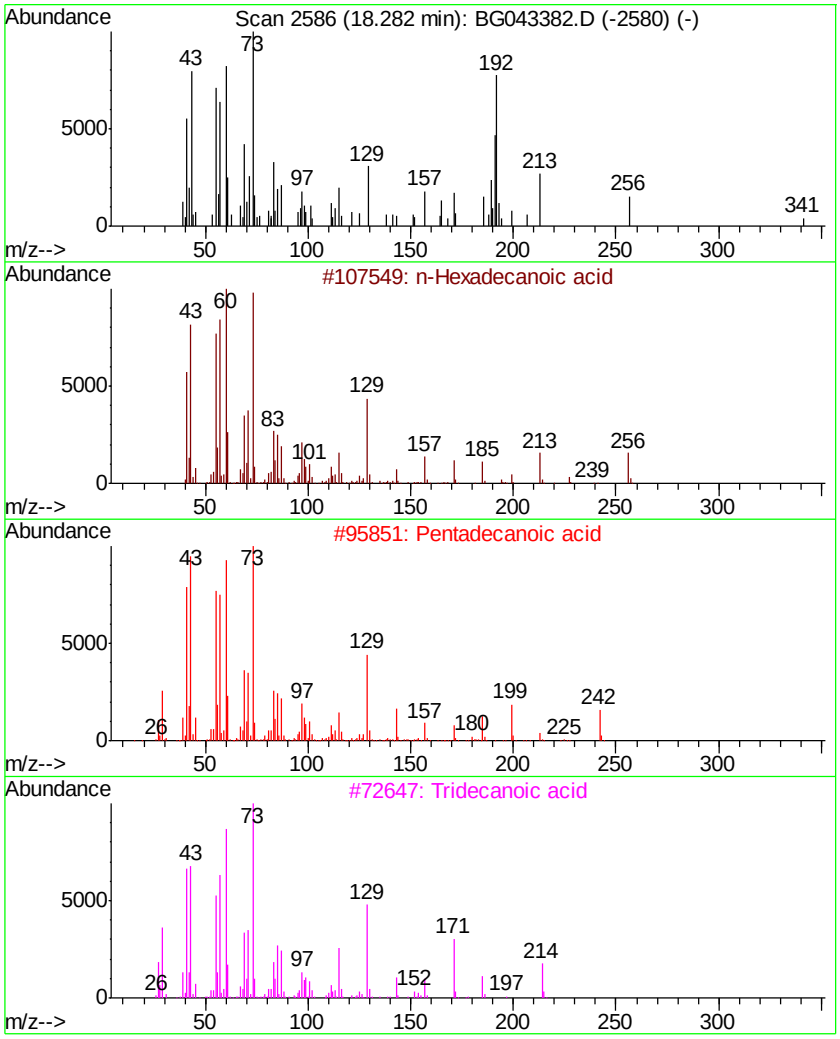
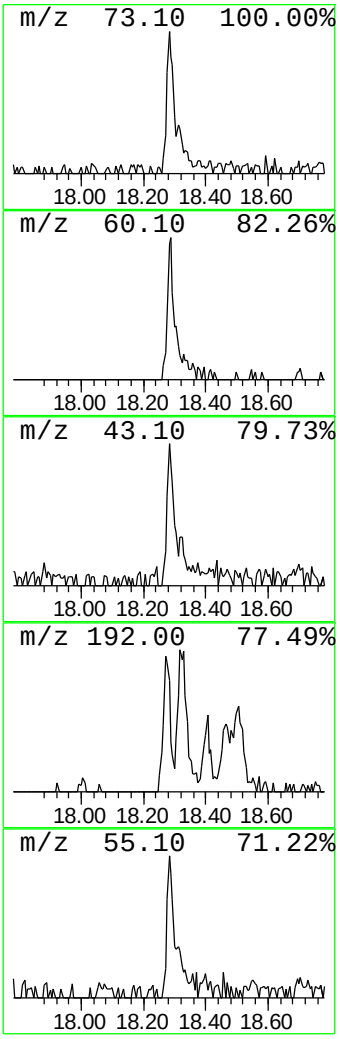
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.58 ng	86647	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
3	Tridecanoic acid	214	C13H26O2	000638-53-9	43
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
Sample : K5541-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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

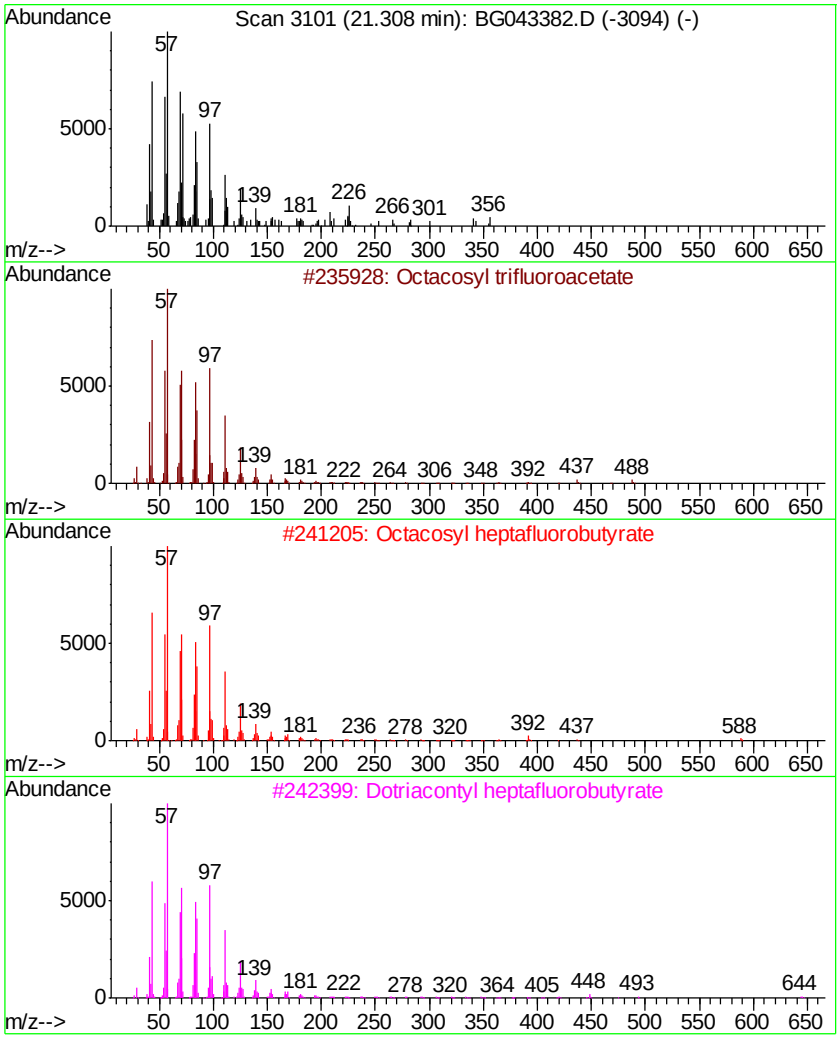
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

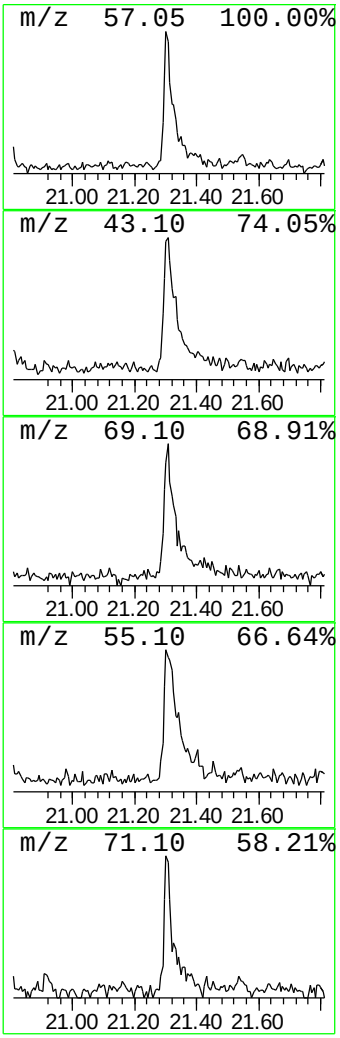
****

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.48 ng	130310	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	93
2	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	93
3	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	93
4	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	87
5	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	87





Library Search Compound Report

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-20-(0-2.5)

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

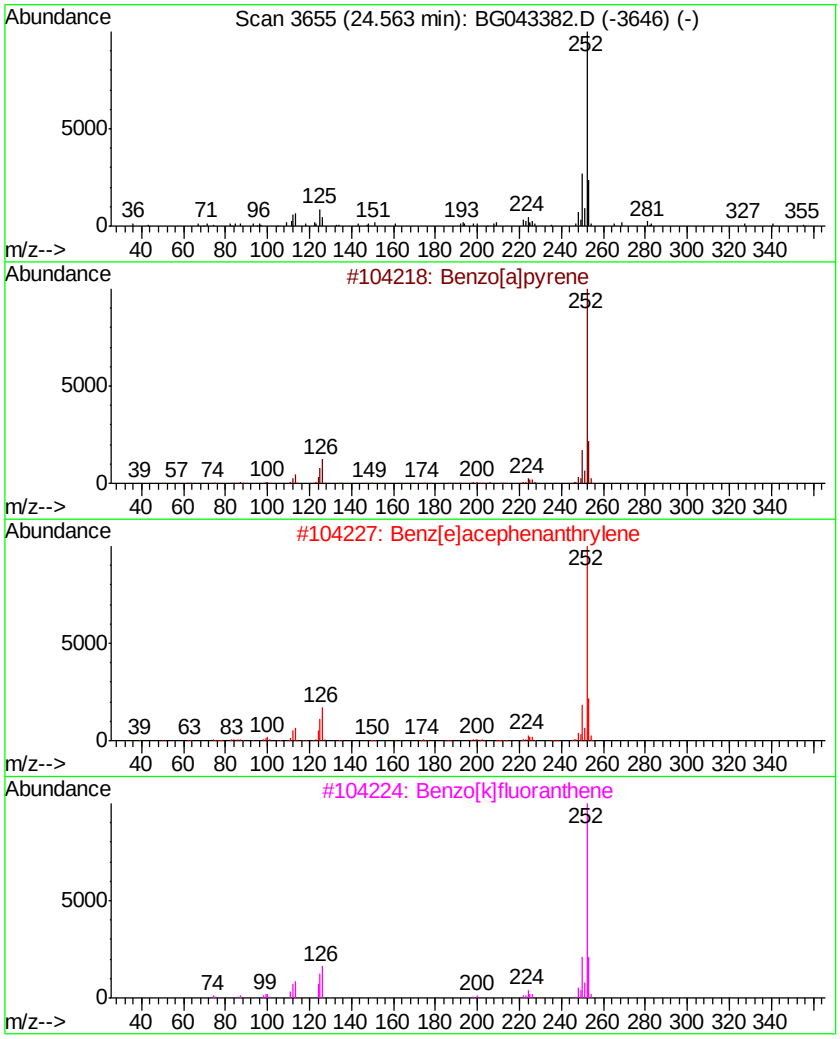
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

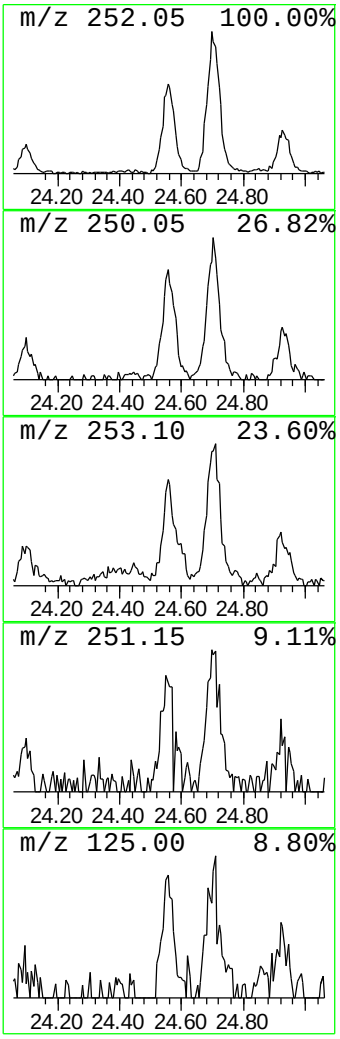
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.56	2.19 ng	107205	Perylene-d12	24.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	81
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
4	Perylene	252	C20H12	000198-55-0	72
5	Benzo[e]pyrene	252	C20H12	000192-97-2	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102919\
Data File : BG043382.D
Acq On : 29 Oct 2019 20:15
Operator : JU
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Instrument : BNA_G
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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	12.9	ng	173384	1	8.02	268193	20.0
2-Pentanone, 4-hy...	5.13	11.5	ng	154236	1	8.02	268193	20.0
unknown7.56	7.56	71.3	ng	956021	1	8.02	268193	20.0
n-Hexadecanoic acid	18.28	2.6	ng	86647	4	17.39	670790	20.0
Octacosyl trifluo...	21.31	2.5	ng	130310	5	21.66	1051430	20.0
Benzo[e]pyrene	24.56	2.2	ng	107205	6	24.86	977516	20.0