LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012021\
Data File : BG047940.D
Acq On : 20 Jan 2021 16:53
Operator : CG/JU
Sample : M1160-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BASIN-4

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-BG012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047940.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.704	396	403	411	rBV	733831	1152069	38.42%	8.041%
2	7.291	663	673	684	rBV	748710	1272009	42.42%	8.878%
3	8.149	812	819	828	rBV	166725	279072	9.31%	1.948%
4	9.312	1008	1017	1026	rBV	435411	744746	24.84%	5.198%
5	10.963	1287	1298	1306	rBV	209926	382389	12.75%	2.669%
6	13.401	1706	1713	1720	rVB	1089784	1659798	55.35%	11.585%
7	14.218	1841	1852	1858	rBV	70016	125652	4.19%	0.877%
8	14.735	1934	1940	1942	rBV2	108112	149788	5.00%	1.045%
9	14.770	1942	1946	1953	rVV	356034	547383	18.25%	3.821%
10	14.841	1953	1958	1968	rVB2	23055	39147	1.31%	0.273%
11	15.029	1983	1990	1996	rBV2	45323	67504	2.25%	0.471%
12	16.251	2186	2198	2208	rBV	897033	1429675	47.68%	9.979%
13	16.333	2208	2212	2221	rVB3	46472	79425	2.65%	0.554%
14	17.514	2406	2413	2419	rBV	493333	722862	24.11%	5.045%
15	18.396	2558	2563	2571	rBV2	95385	130297	4.35%	0.909%
16	19.547	2755	2759	2768	rVB6	20180	39875	1.33%	0.278%
17	19.659	2774	2778	2785	rBV3	30887	41781	1.39%	0.292%
18	20.117	2850	2856	2862	rVB	2340577	2998693	100.00%	20.930%
19	21.245	3042	3048	3054	rBV	79281	106525	3.55%	0.744%
20	21.433	3076	3080	3092	rBV	111066	191905	6.40%	1.339%
21	21.797	3135	3142	3149	rBV	562907	930776	31.04%	6.497%
22	22.655	3281	3288	3296	rBV4	34012	76463	2.55%	0.534%
23	24.212	3546	3553	3561	rBV2	53025	123442	4.12%	0.862%
24	25.099	3692	3704	3717	rBV2	298561	891523	29.73%	6.223%
25	26.392	3913	3924	3933	rBV5	30393	98070	3.27%	0.685%
26	30.669	4643	4652	4654	rBV9	16760	46272	1.54%	0.323%

Sum of corrected areas: 14327141

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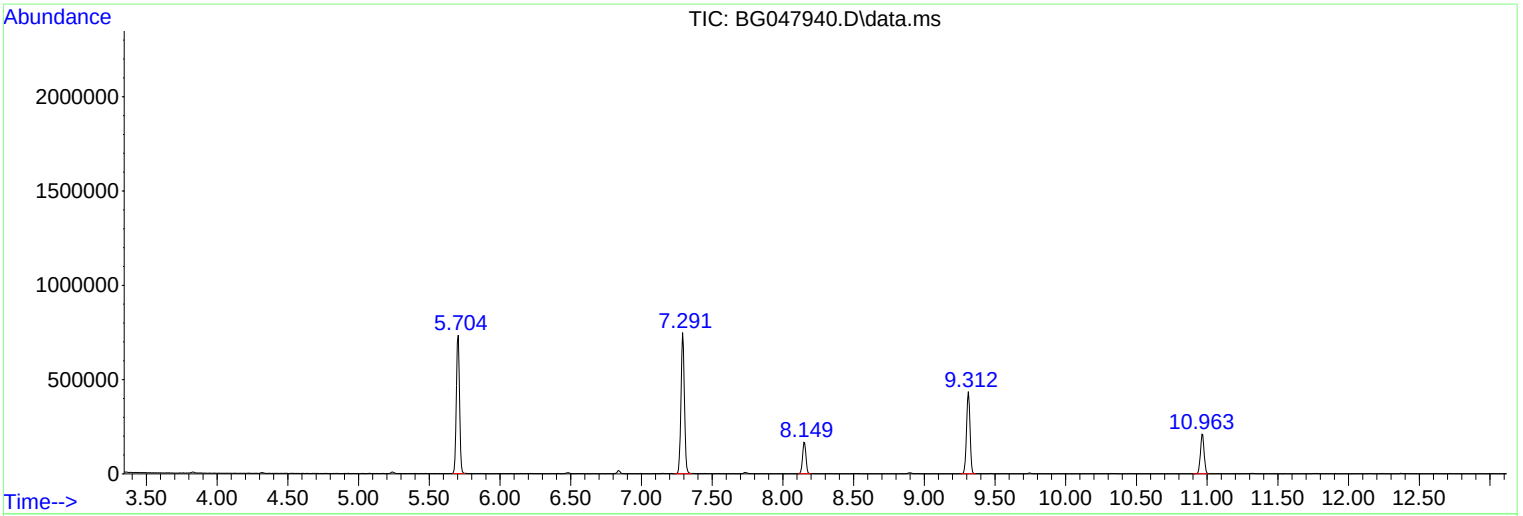
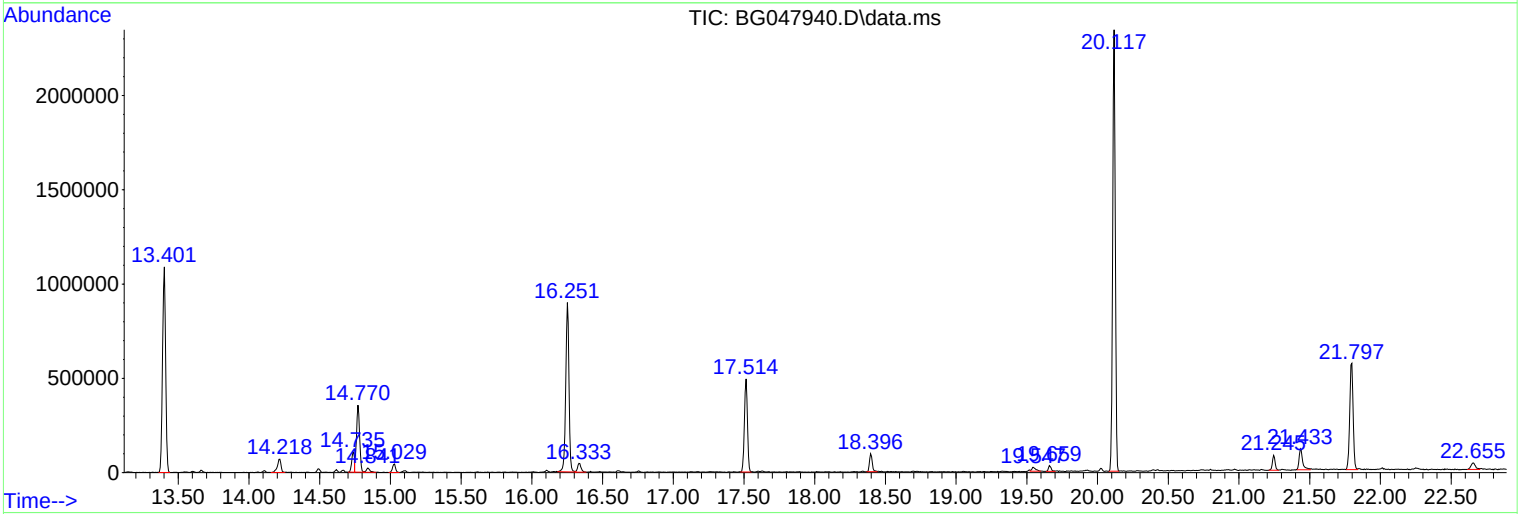
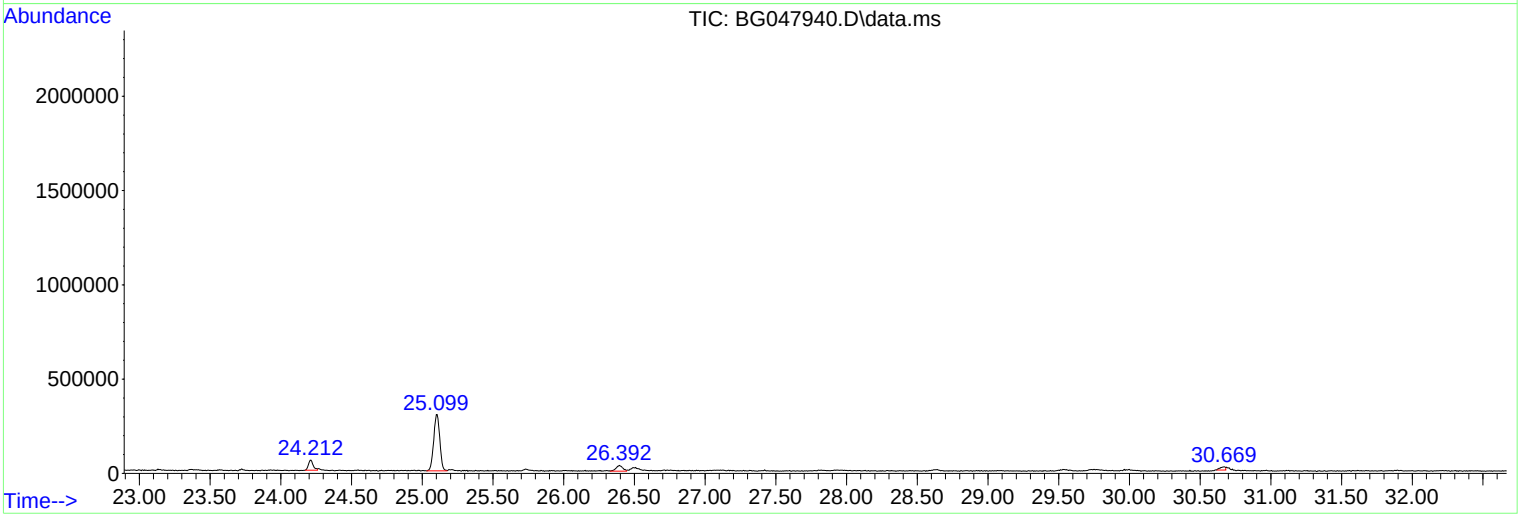
Instrument :
BNA_G
ClientSampleId :
BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.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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ClientSampleId :
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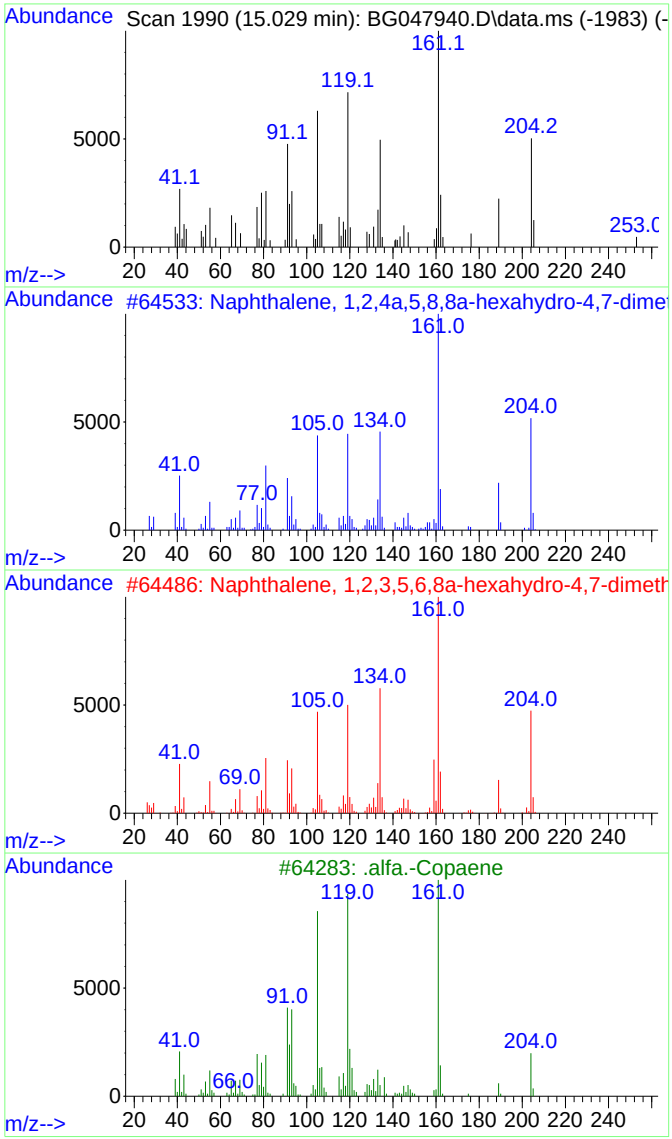
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

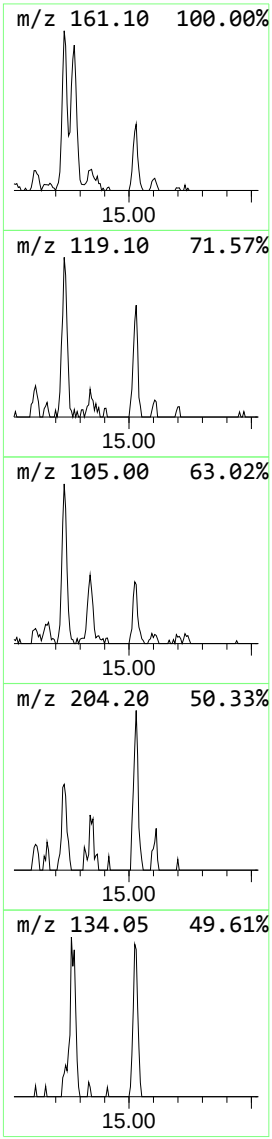
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Naphthalene, 1,2,4a,5,8,8a-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.029	2.47 ng	67504	Acenaphthene-d10	14.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	93
2	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	90
3	.alfa.-Copaene	204	C15H24	1000360-33-0	86
4	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	78
5	Copaene	204	C15H24	003856-25-5	68





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Data File : BG047940.D
Acq On : 20 Jan 2021 16:53
Operator : CG/JU
Sample : M1160-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

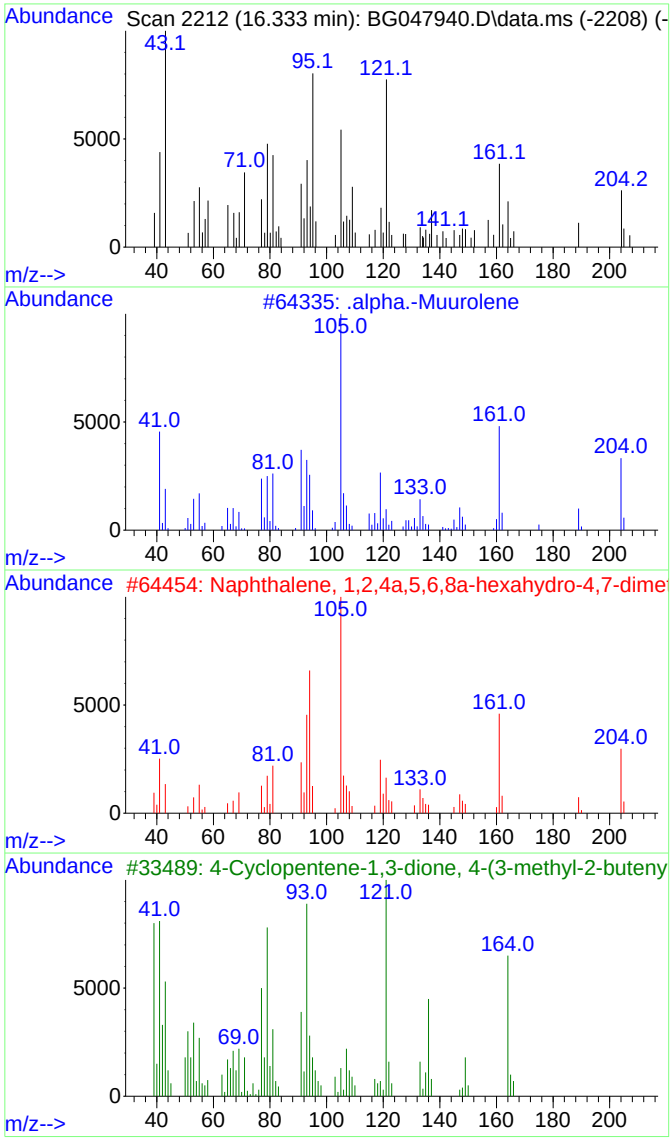
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

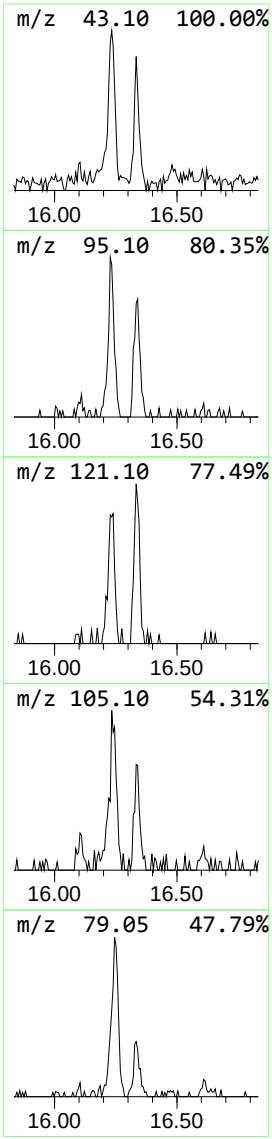
****

Peak Number 2 .alpha.-Muurolene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	2.20 ng	79425	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Muurolene	204	C15H24	031983-22-9	62
2	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	38
3	4-Cyclopentene-1,3-dione, 4-(3-m...	164	C10H12O2	058940-75-3	35
4	.tau.-Muurolol	222	C15H26O	019912-62-0	27
5	trans-7-Carboxy-bicyclo[4.3.0]no...	166	C10H14O2	070071-94-2	25





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Data File : BG047940.D
Acq On : 20 Jan 2021 16:53
Operator : CG/JU
Sample : M1160-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

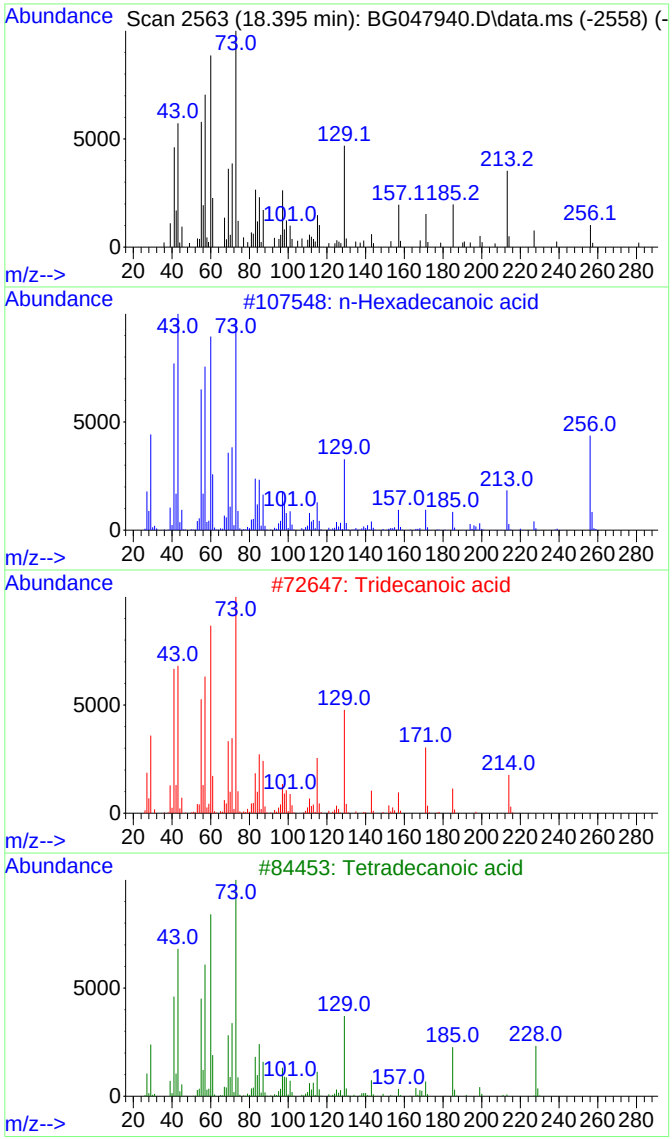
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

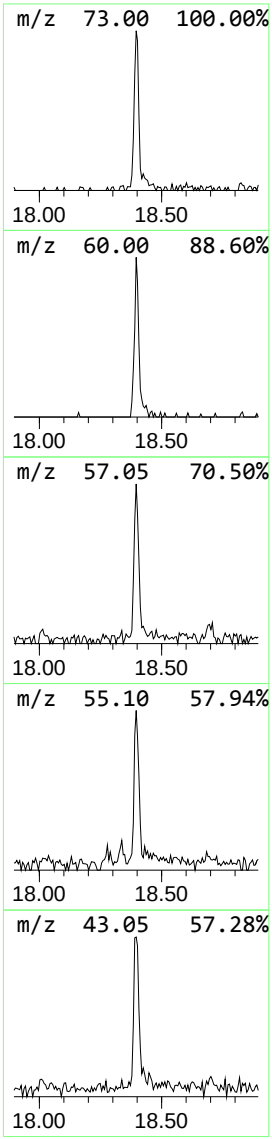
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.395	3.61 ng	130297	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





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Data File : BG047940.D
Acq On : 20 Jan 2021 16:53
Operator : CG/JU
Sample : M1160-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

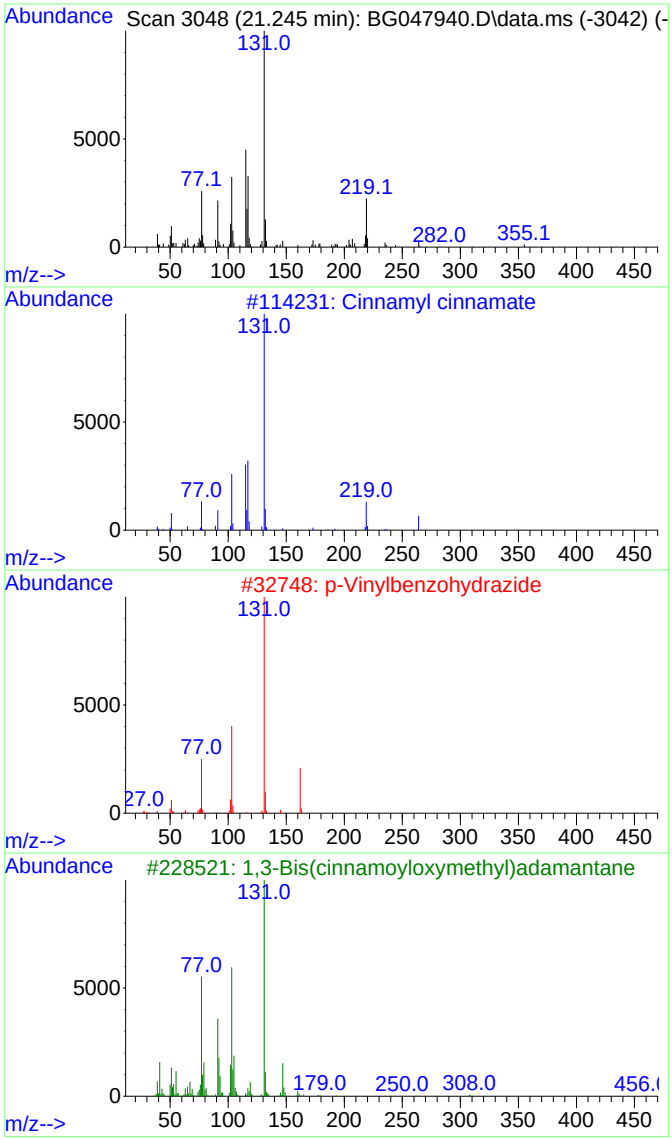
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

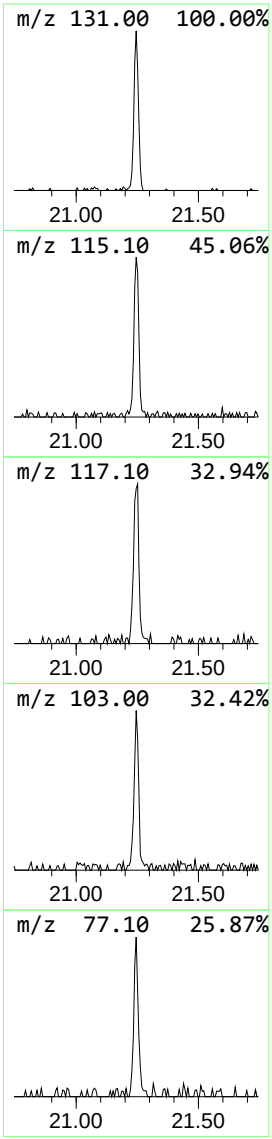
****

Peak Number 4 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	2.29 ng	106525	Chrysene-d12	21.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	78
2	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	47
3	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47
4	Oxalic acid, monoamide monohydra...	323	C18H17N3O3	1000294-01-4	47
5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47





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Sample : M1160-09
Misc :
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Instrument :
BNA_G
ClientSampleId :
BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
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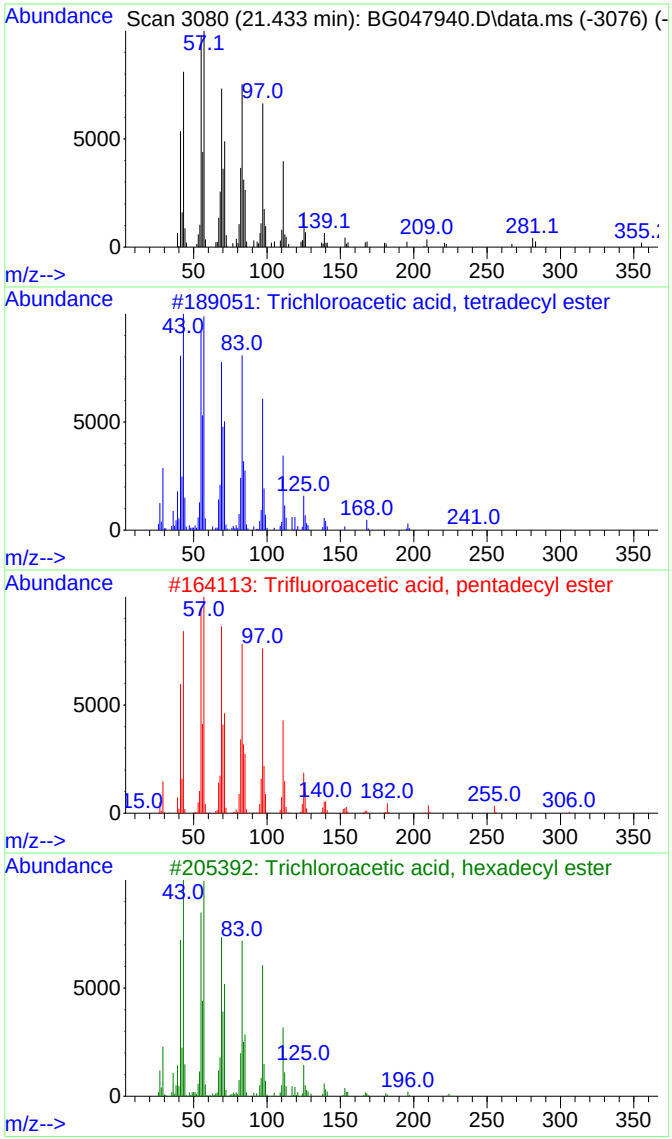
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

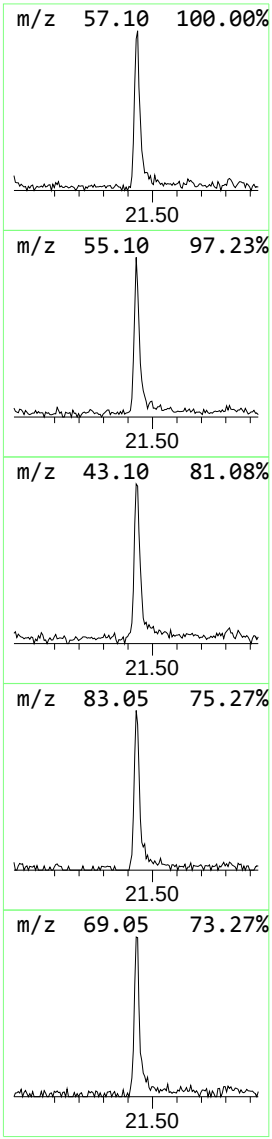
****

Peak Number 5 Trichloroacetic acid, tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.433	4.12 ng	191905	Chrysene-d12	21.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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TIC Library : C:\Database\NIST11.L
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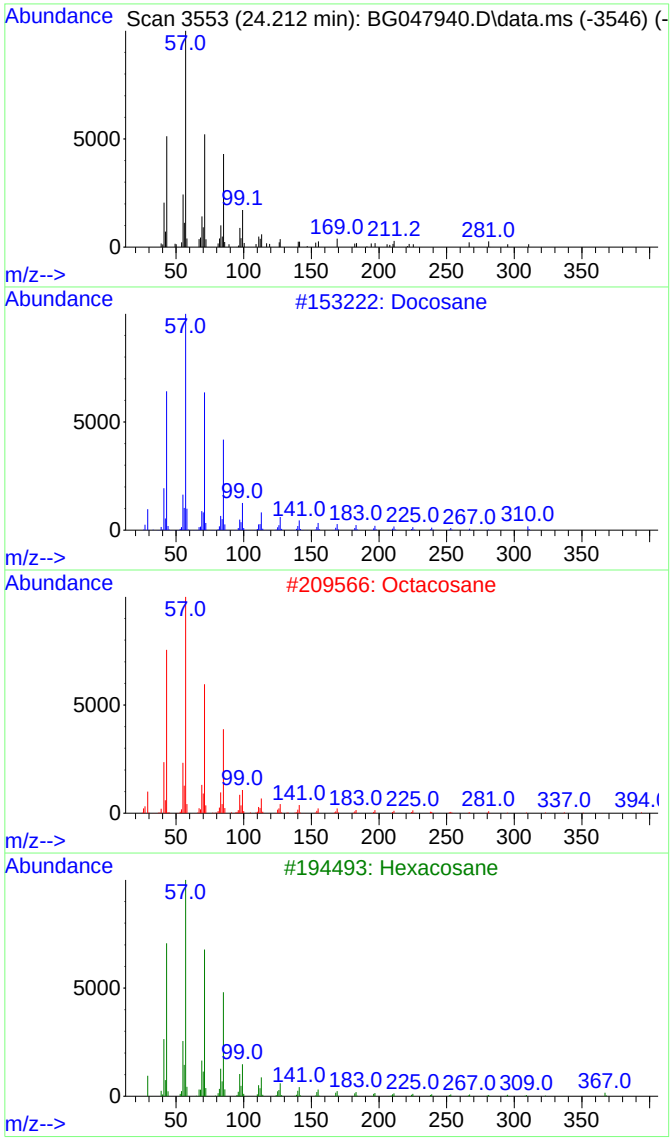
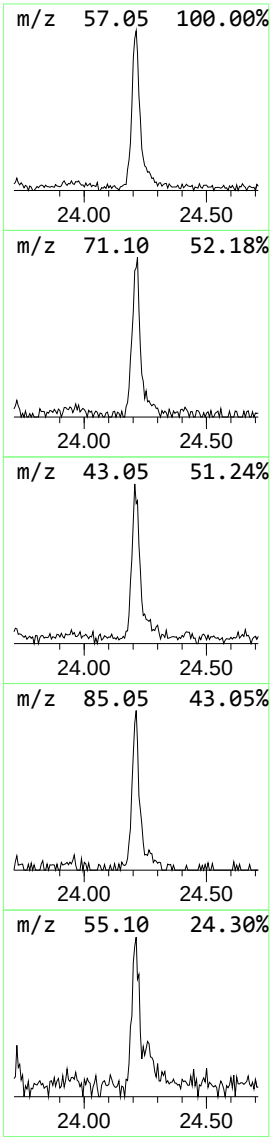
****

Peak Number 6 Docosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.212	2.77 ng	123442	Perylene-d12	25.099

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Octacosane	394	C28H58	000630-02-4	83
3	Hexacosane	366	C26H54	000630-01-3	81
4	Eicosane	282	C20H42	000112-95-8	80
5	Hentriacontane	437	C31H64	000630-04-6	80





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BASIN-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

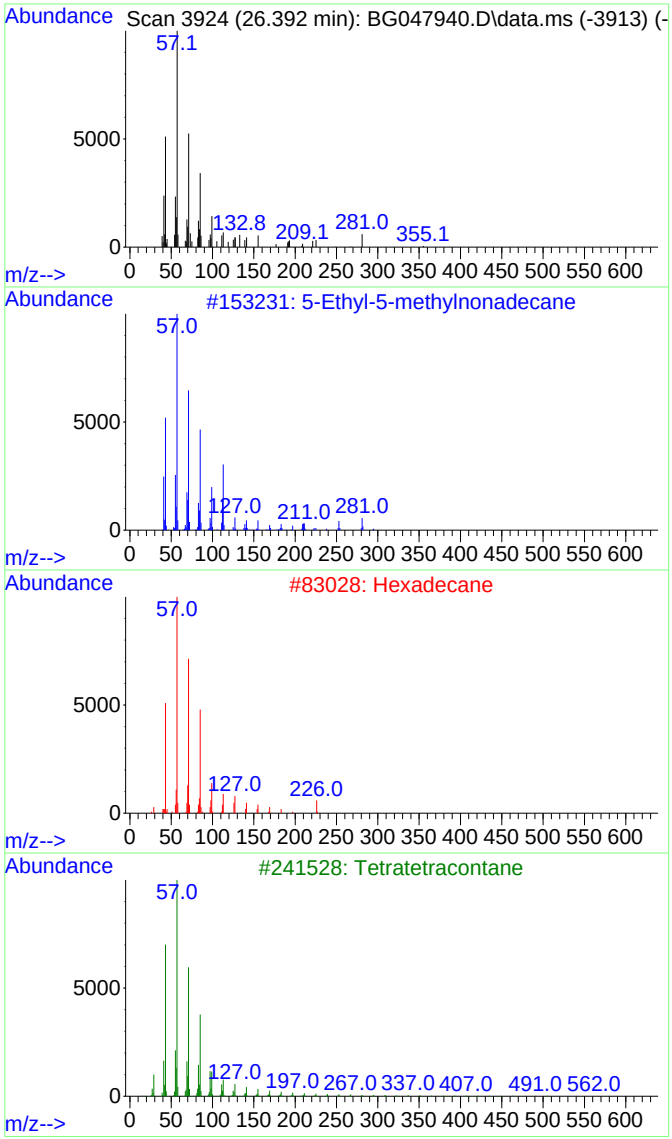
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

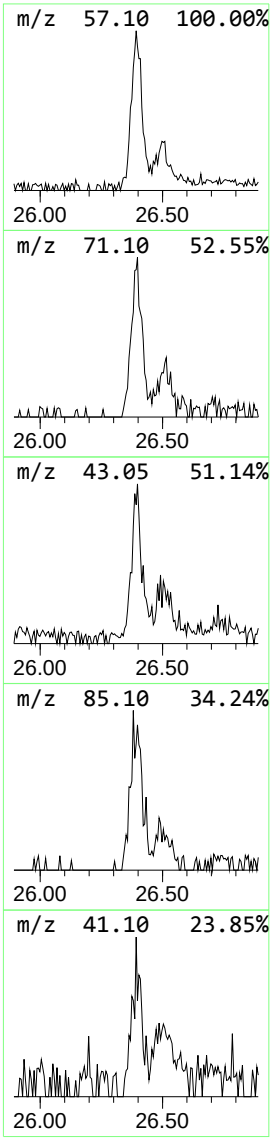
****

Peak Number 7 5-Ethyl-5-methylnonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.392	2.20 ng	98070	Perylene-d12	25.099

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	87
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Heptadecane	240	C17H36	000629-78-7	86





Tentatively Identified Compound (LSC) summary

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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
Naphthalene, 1,...	15.029	2.5	ng	67504	3	14.770	547383	20.0
.alpha.-Muurolene	16.333	2.2	ng	79425	4	17.514	722862	20.0
n-Hexadecanoic ...	18.395	3.6	ng	130297	4	17.514	722862	20.0
Cinnamyl cinnamate	21.245	2.3	ng	106525	5	21.797	930776	20.0
Trichloroacetic...	21.433	4.1	ng	191905	5	21.797	930776	20.0
Docosane	24.212	2.8	ng	123442	6	25.099	891523	20.0
5-Ethyl-5-methy...	26.392	2.2	ng	98070	6	25.099	891523	20.0