LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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	3.171	9	14	29	rVB	613912	947068	29.84%	6.939%
2	5.116	338	345	354	rBV	48023	82332	2.59%	0.603%
3	5.598	420	427	443	rBV	299465	542134	17.08%	3.972%
4	7.196	692	699	709	rBV	189549	383156	12.07%	2.807%
5	7.548	752	759	771	rBV	466233	872277	27.49%	6.391%
6	8.012	830	838	847	rBV	103585	189351	5.97%	1.387%
7	8.336	886	893	903	rBV	356227	645298	20.33%	4.728%
8	9.176	1027	1036	1050	rBV	243765	518582	16.34%	3.799%
9	10.815	1307	1315	1329	rBV	109002	236271	7.44%	1.731%
10	13.265	1725	1732	1744	rBV	736575	1294135	40.78%	9.482%
11	14.640	1960	1966	1981	rBV	217625	385659	12.15%	2.826%
12	16.132	2213	2220	2238	rBV	748766	1348351	42.49%	9.879%
13	17.390	2427	2434	2446	rBV	294411	528467	16.65%	3.872%
14	18.277	2580	2585	2594	rBV4	25562	53595	1.69%	0.393%
15	19.998	2872	2878	2891	rBV	2370806	3173607	100.00%	23.252%
16	21.297	3095	3099	3107	rVV4	50940	127260	4.01%	0.932%
17	21.379	3109	3113	3123	rVB	42519	94219	2.97%	0.690%
18	21.655	3152	3160	3169	rBV	427302	825661	26.02%	6.049%
19	21.837	3188	3191	3204	rVB3	49309	87074	2.74%	0.638%
20	22.443	3290	3294	3299	rVB3	44902	70315	2.22%	0.515%
21	23.124	3404	3410	3418	rBV3	53513	107186	3.38%	0.785%
22	23.923	3540	3546	3554	rVB3	51368	109970	3.47%	0.806%
23	24.857	3693	3705	3719	rBV	298972	916438	28.88%	6.714%
24	25.974	3891	3895	3905	rVB6	45003	110531	3.48%	0.810%

Sum of corrected areas: 13648937

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
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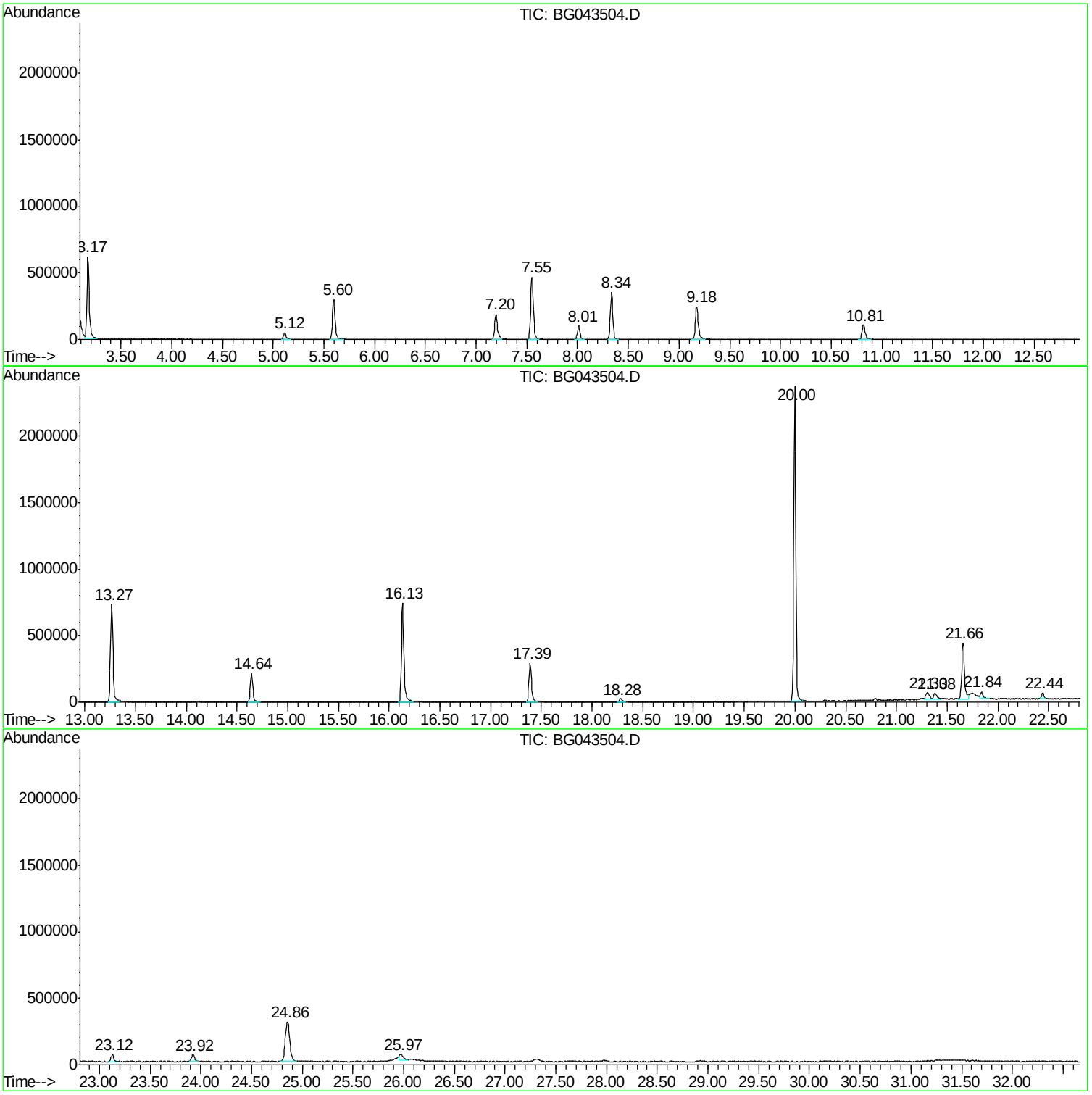
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB124540BL

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId : PB124540BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

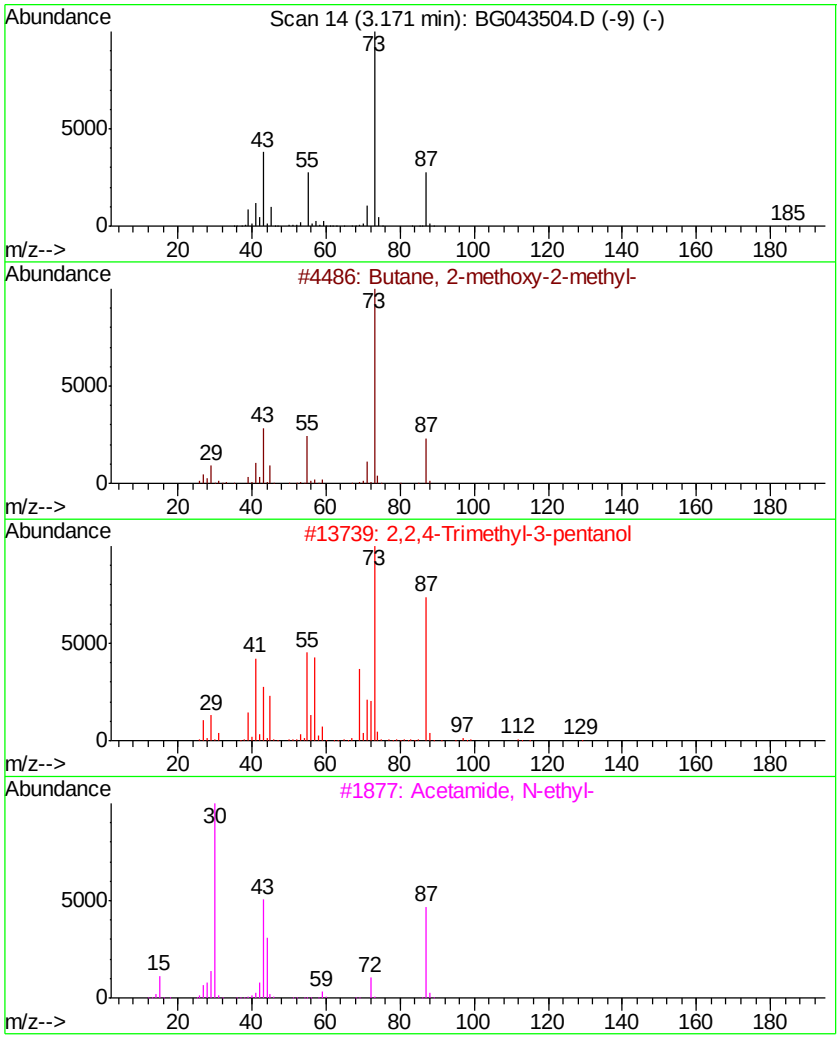
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

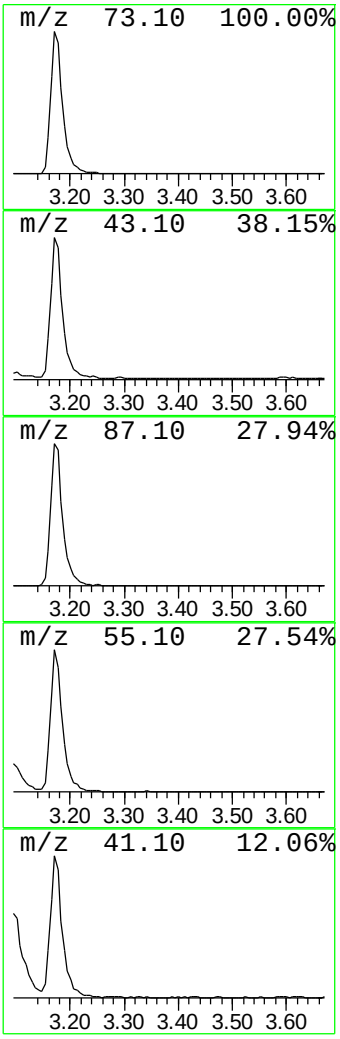
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	100.03 ng	947068	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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

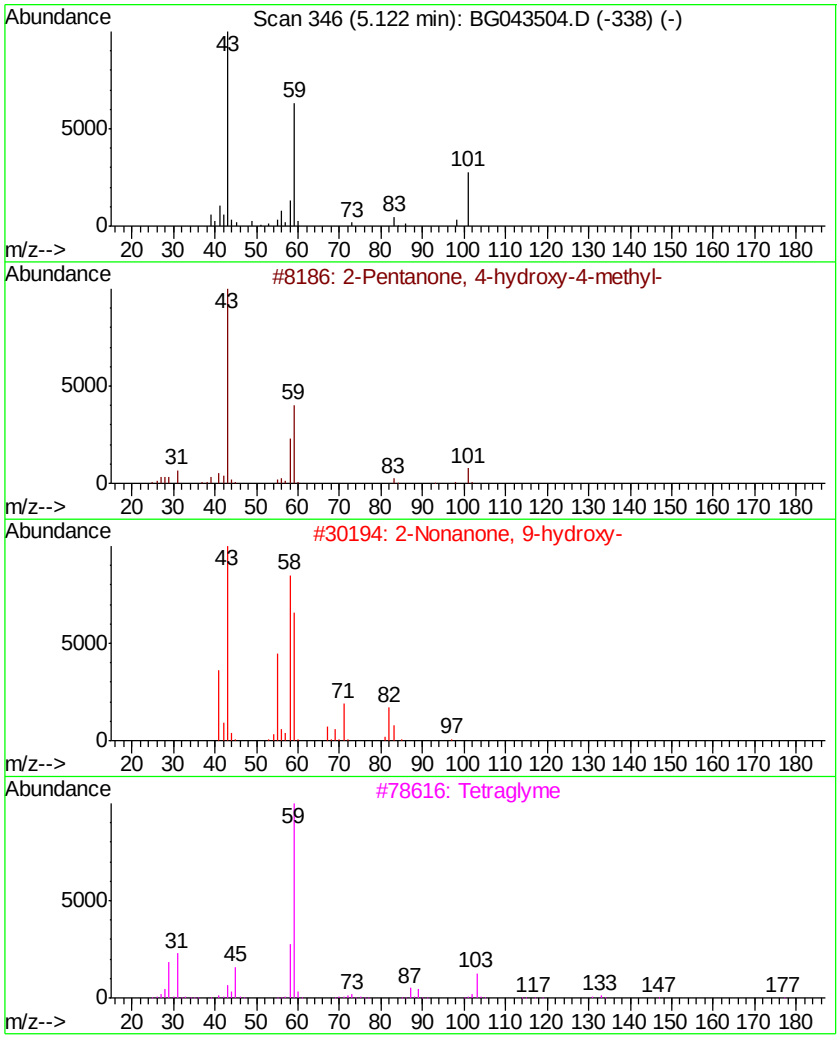
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

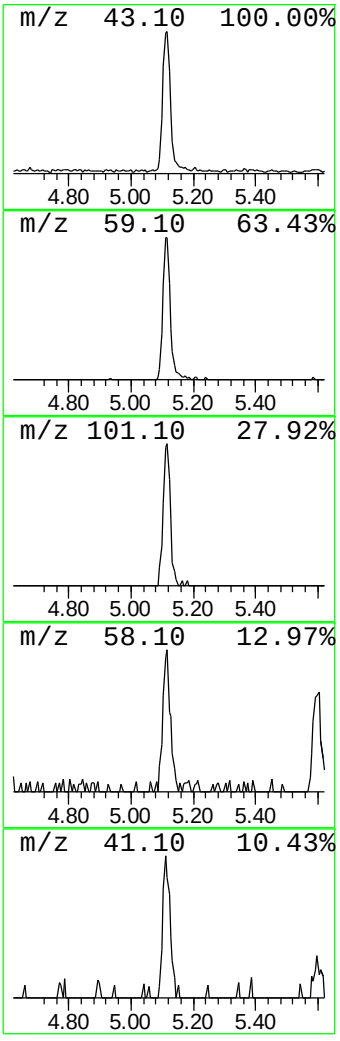
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	8.70 ng	82332	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	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
3	Tetraglyme	222	C10H22O5	000143-24-8	25
4	Pentanal, oxime	101	C5H11NO	000628-79-5	23
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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

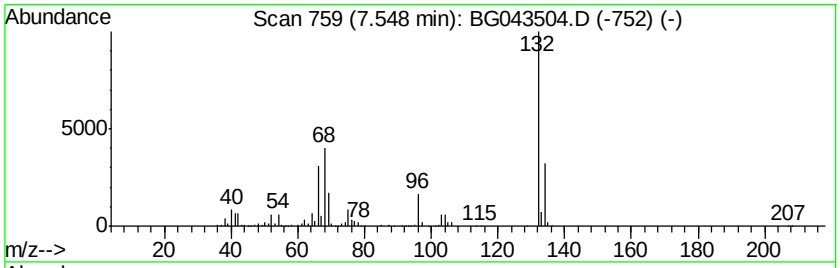
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

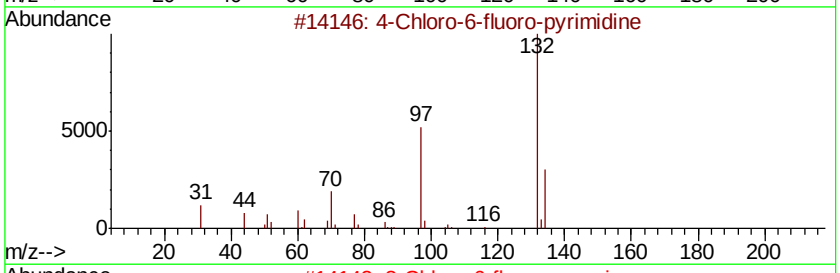
****

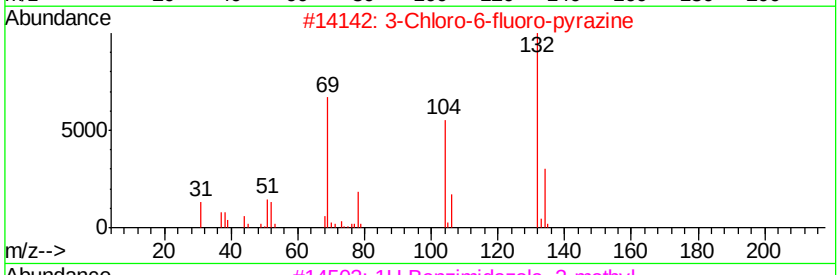
Peak Number 3 unknown7.55 Concentration Rank 2

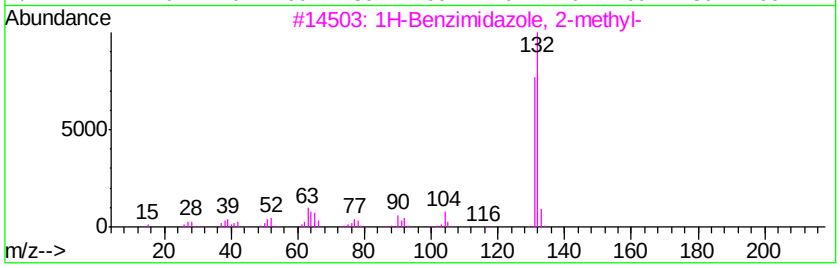
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	92.13 ng	872277	1,4-Dichlorobenzene-d4	8.01

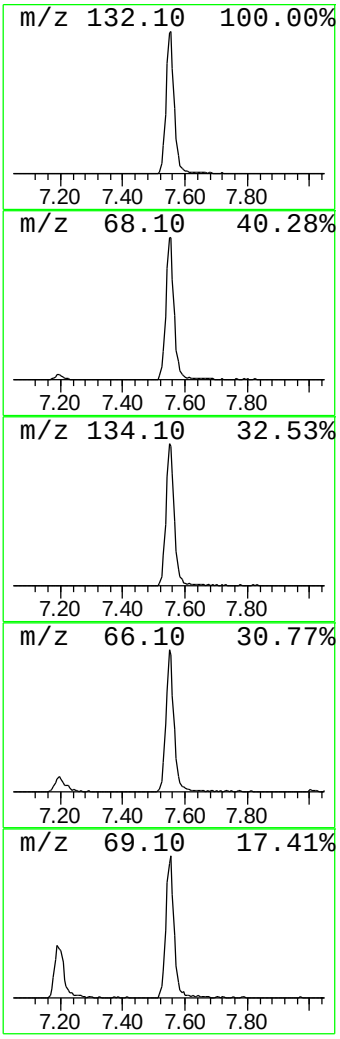
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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

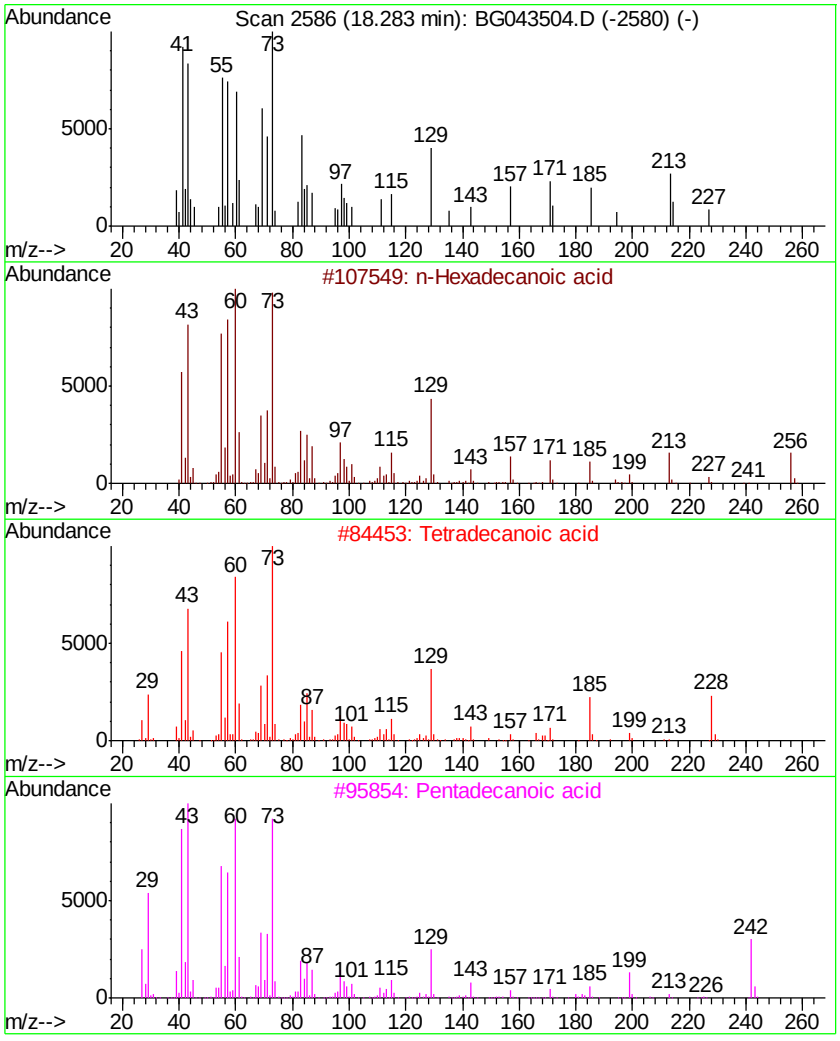
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

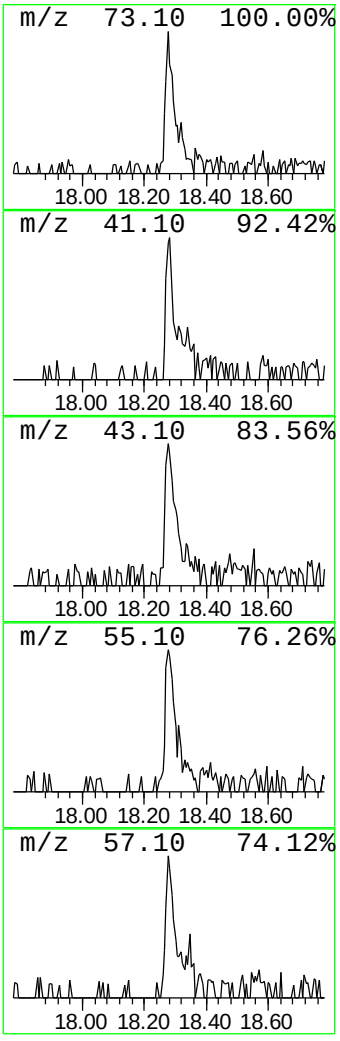
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.03 ng	53595	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	Tridecanoic acid	214	C13H26O2	000638-53-9	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
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Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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
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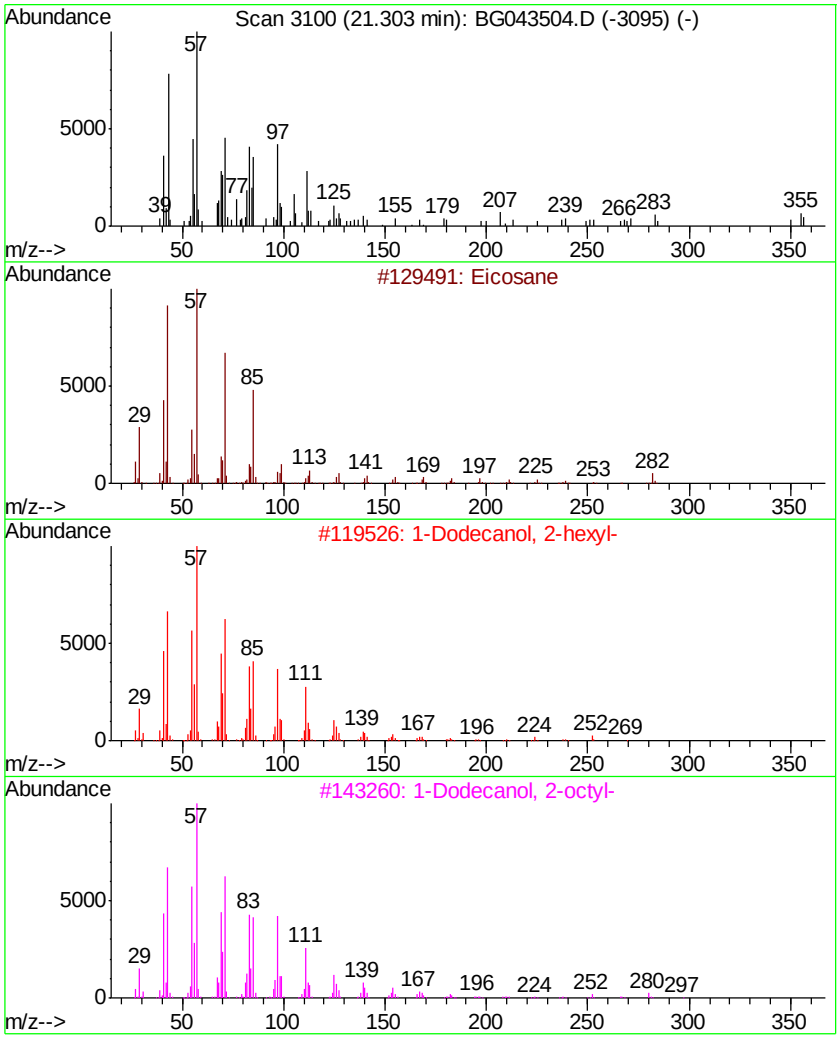
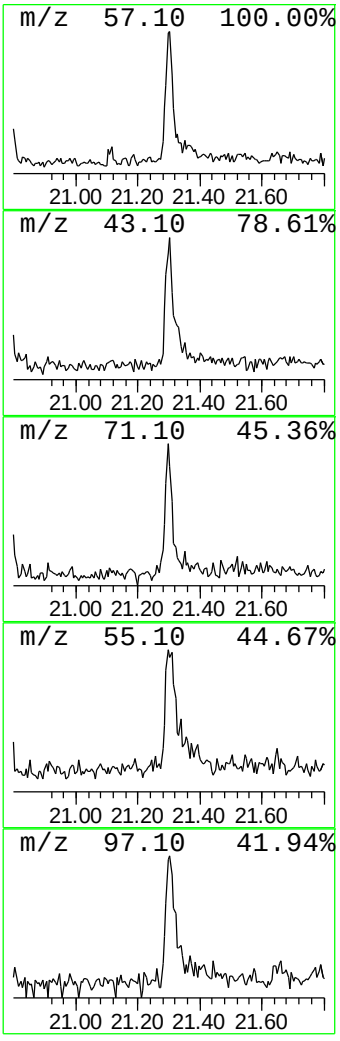
****

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	3.08 ng	127260	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
4	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	83
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	80





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Instrument : BNA_G
ClientSampleId : PB124540BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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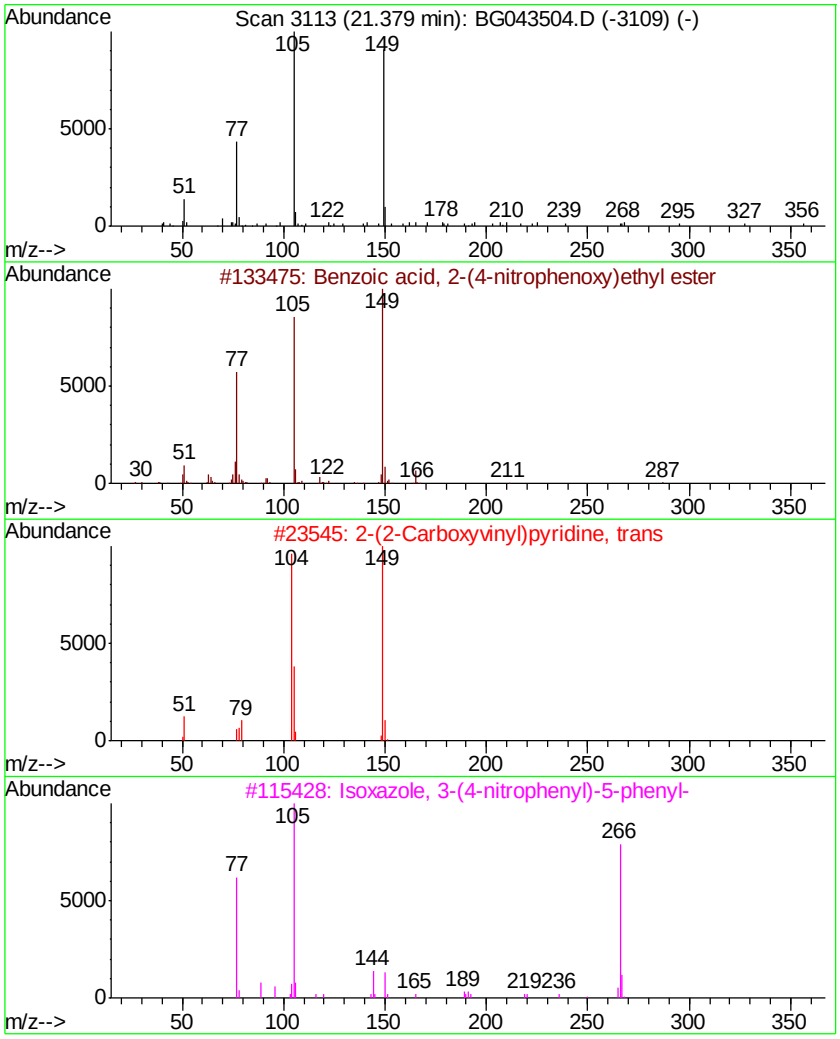
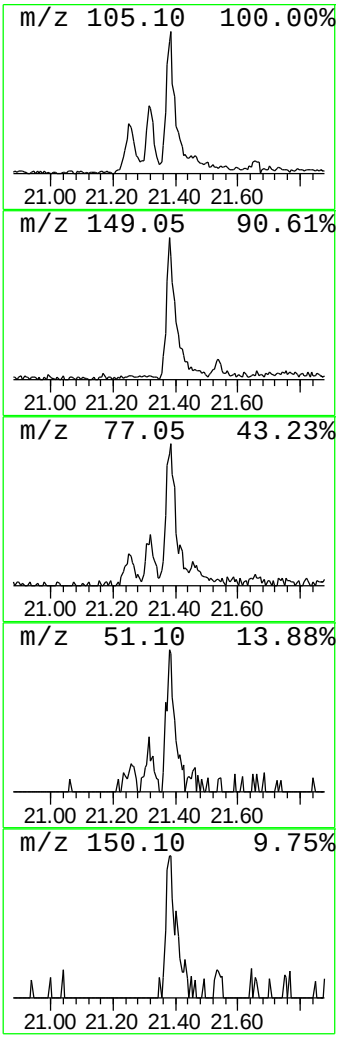
****

Peak Number 7 Benzoic acid, 2-(4-nitrophe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	2.28 ng	94219	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
2	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	53
3	Isoxazole, 3-(4-nitrophenyl)-5-p...	266	C15H10N2O3	031108-56-2	27
4	N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	27
5	.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	22





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Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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
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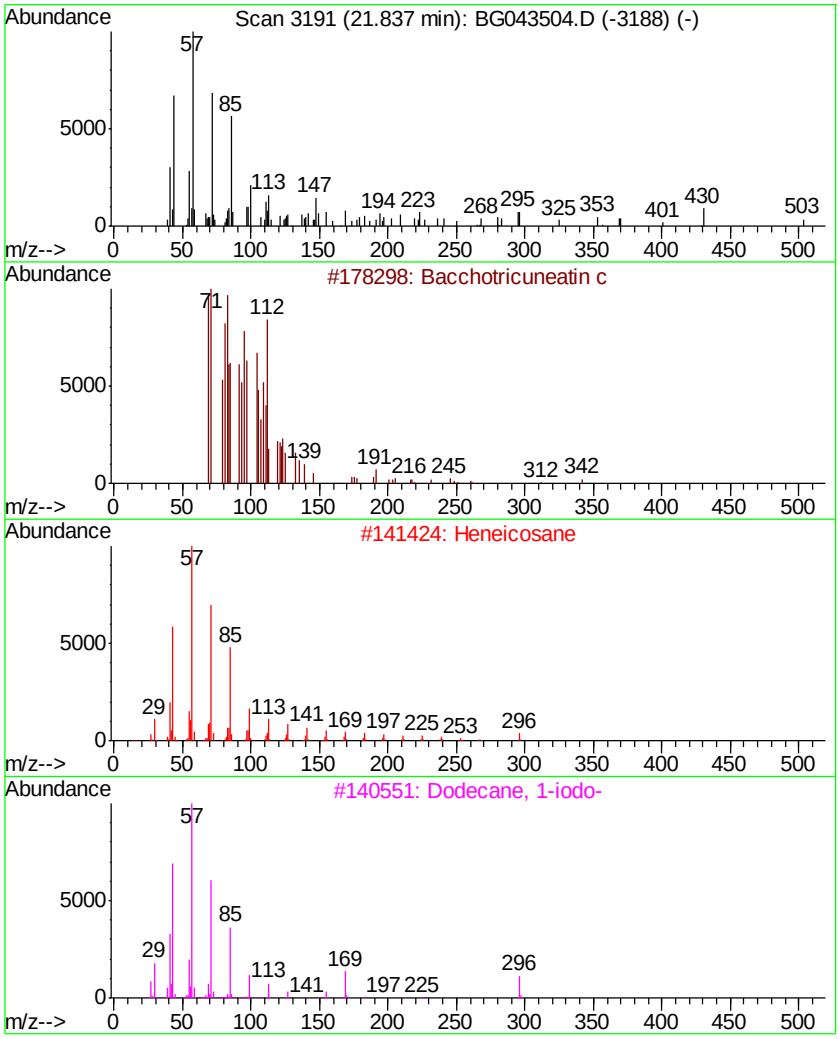
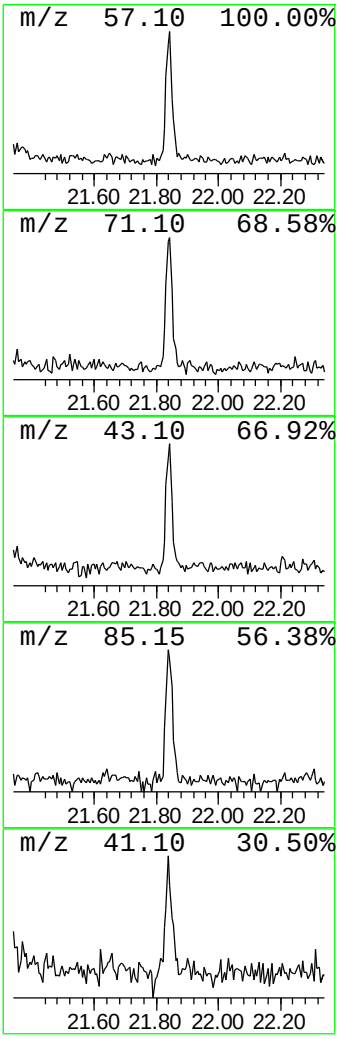
****

Peak Number 8 Bacchotricuneatin c Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	2.11 ng	87074	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	97
2	Heneicosane	296	C21H44	000629-94-7	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	81
4	Nonadecane	268	C19H40	000629-92-5	76
5	Tetracosane	338	C24H50	000646-31-1	68





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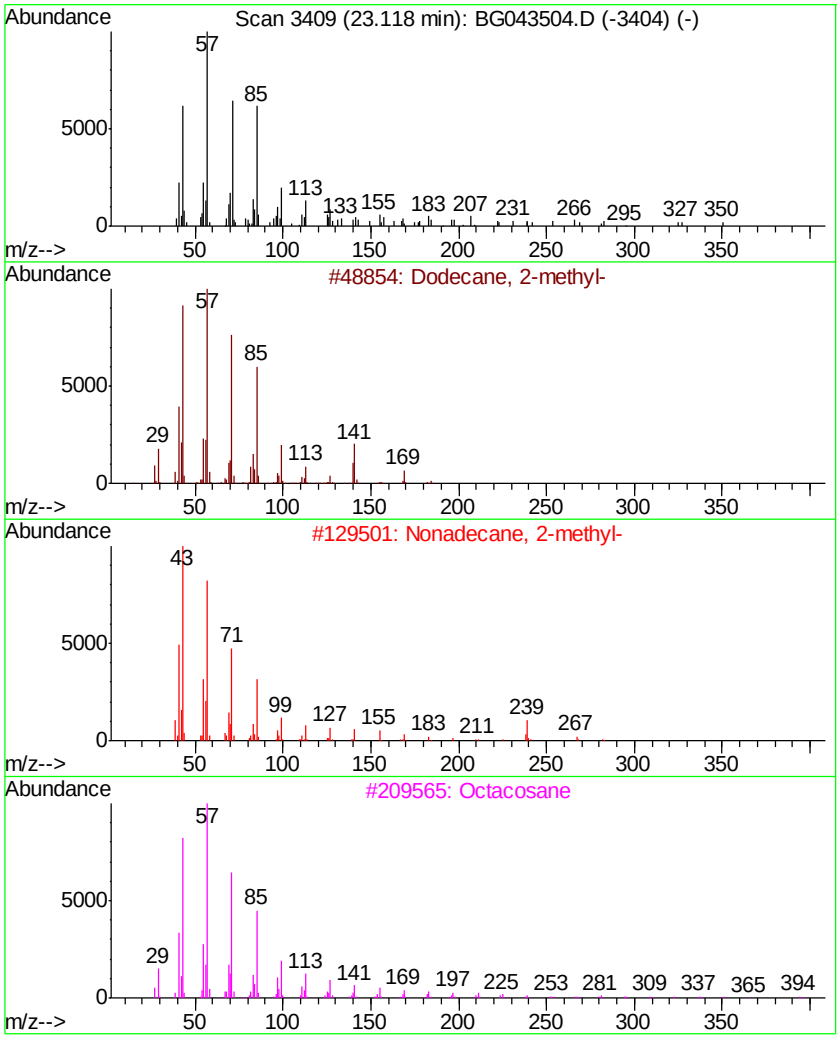
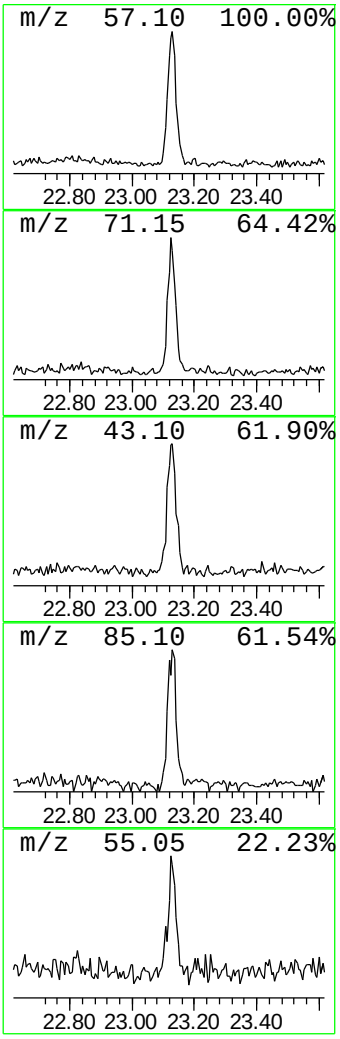
****

Peak Number 9 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	2.60 ng	107186	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Triacontane	422	C30H62	000638-68-6	87
5	Heneicosane	296	C21H44	000629-94-7	83





Library Search Compound Report

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Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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
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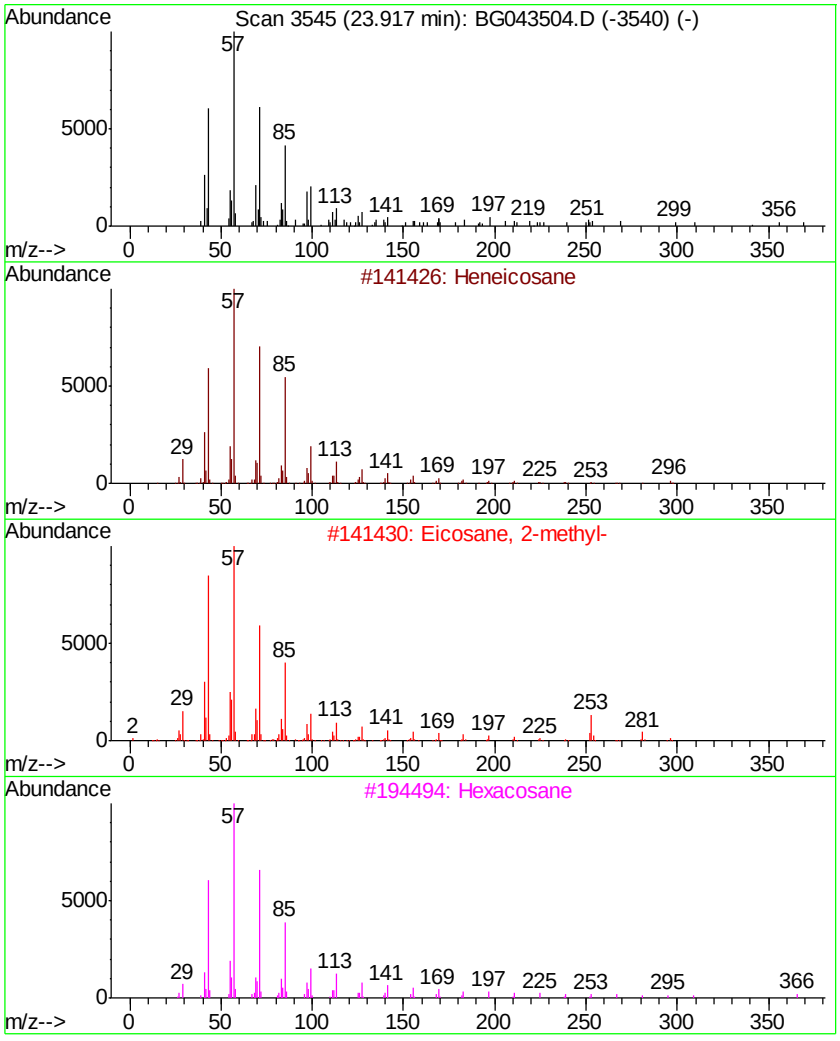
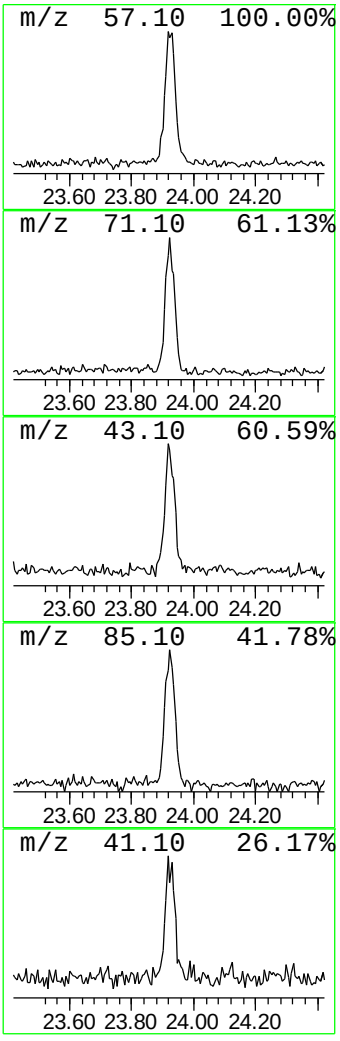
****

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	2.40 ng	109970	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	94
3	Hexacosane	366	C26H54	000630-01-3	93
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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

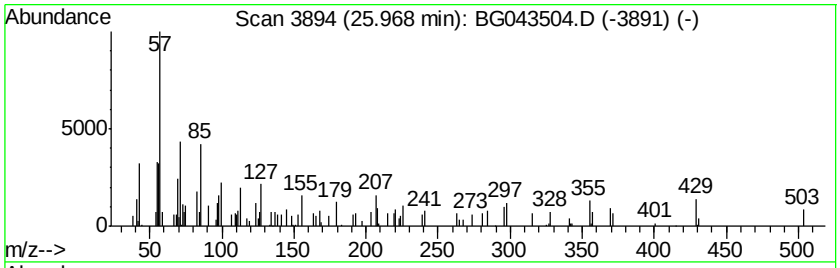
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

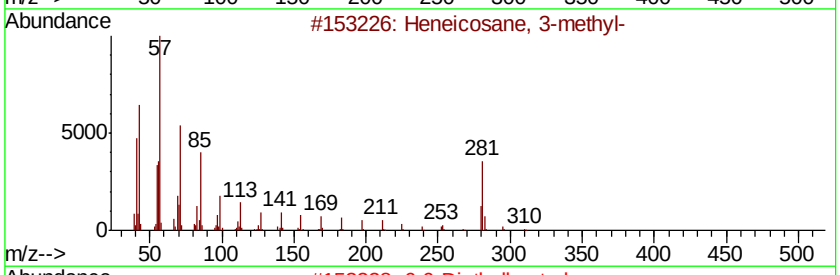
****

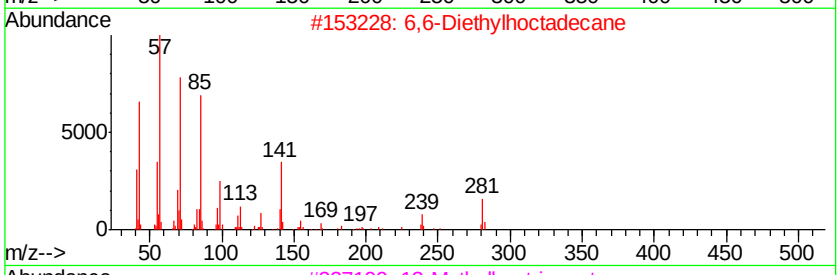
Peak Number 11 unknown25.97 Concentration Rank 7

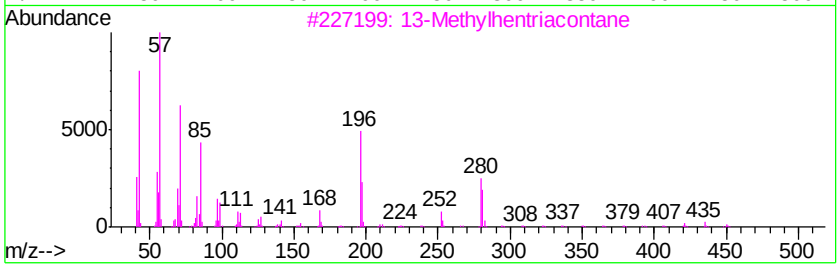
R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	2.41 ng	110531	Perylene-d12	24.85

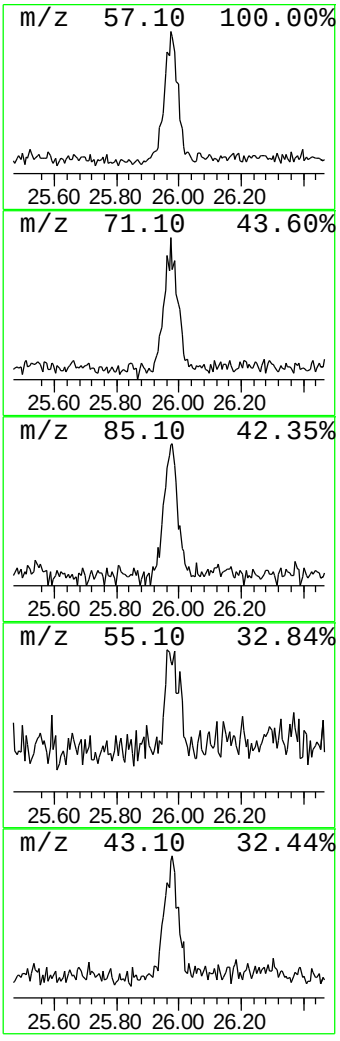
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 3-methyl-	310	C22H46	006418-47-9	38
2	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	32
3	13-Methylhentriacontane	451	C32H66	1000131-19-4	12
4	Tetra(diethylamino)vanadium	339	C16H40N4V	1000102-48-5	10
5	Octadecane, 9-ethyl-9-heptyl-	380	C27H56	055282-27-4	9











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110519\
Data File : BG043504.D
Acq On : 5 Nov 2019 12:41
Operator : JU
Sample : PB124540BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124540BL

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...	3.17	100.0	ng	947068	1	8.01	189351	20.0
2-Pentanone, 4-hy...	5.12	8.7	ng	82332	1	8.01	189351	20.0
unknown7.55	7.55	92.1	ng	872277	1	8.01	189351	20.0
n-Hexadecanoic acid	18.28	2.0	ng	53595	4	17.39	528467	20.0
Eicosane	21.30	3.1	ng	127260	5	21.66	825661	20.0
Benzoic acid, 2-(...	21.38	2.3	ng	94219	5	21.66	825661	20.0
Bacchotricuneatin c	21.84	2.1	ng	87074	5	21.66	825661	20.0
Dodecane, 2-methyl-	23.12	2.6	ng	107186	5	21.66	825661	20.0
Heneicosane	23.92	2.4	ng	109970	6	24.85	916438	20.0
unknown25.97	25.97	2.4	ng	110531	6	24.85	916438	20.0