LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

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-BG071519.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	3.191	13	17	30	rVB	562795	873272	13.10%	1.976%
2	3.726	105	108	119	rVB2	39619	69283	1.04%	0.157%
3	5.612	421	429	441	rBV	2052894	3286053	49.29%	7.436%
4	7.204	691	700	711	rBV	2163665	3773622	56.60%	8.540%
5	7.580	756	764	781	rBV	2097934	3585676	53.78%	8.114%
6	8.050	836	844	851	rBV	402428	678154	10.17%	1.535%
7	8.373	891	899	909	rBV	1520737	2640348	39.60%	5.975%
8	9.208	1032	1041	1053	rBV	1254491	2265759	33.99%	5.127%
9	10.859	1312	1322	1330	rBV	536179	992306	14.88%	2.246%
10	12.304	1560	1568	1577	rBV	70361	112815	1.69%	0.255%
11	13.297	1729	1737	1745	rBV	3179497	4906345	73.59%	11.103%
12	14.114	1870	1876	1889	rVB	462237	676934	10.15%	1.532%
13	14.666	1962	1970	1982	rVB2	867853	1394865	20.92%	3.157%
14	16.147	2215	2222	2235	rBV	2700254	3993035	59.90%	9.036%
15	17.404	2429	2436	2445	rBV2	1139765	1720896	25.81%	3.894%
16	18.297	2583	2588	2598	rBV	272328	410131	6.15%	0.928%
17	19.566	2799	2804	2811	rBV	96150	153016	2.30%	0.346%
18	20.007	2873	2879	2885	rBV	4748472	6666710	100.00%	15.087%
19	21.335	3099	3105	3122	rBV3	134314	586787	8.80%	1.328%
20	21.652	3152	3159	3166	rBV2	1128572	1870469	28.06%	4.233%
21	21.881	3194	3198	3202	rVB	70441	94299	1.41%	0.213%
22	22.498	3297	3303	3308	rBV	118650	205235	3.08%	0.464%
23	23.197	3416	3422	3429	rVB	150004	307343	4.61%	0.696%
24	23.385	3449	3454	3462	rVB	60250	128788	1.93%	0.291%
25	24.008	3552	3560	3571	rBV	146237	344789	5.17%	0.780%
26	24.854	3693	3704	3715	rVB2	698971	1935601	29.03%	4.380%
27	24.966	3717	3723	3733	rVB2	109145	286827	4.30%	0.649%
28	26.111	3913	3918	3928	rVB3	79041	229483	3.44%	0.519%

Sum of corrected areas: 44188841

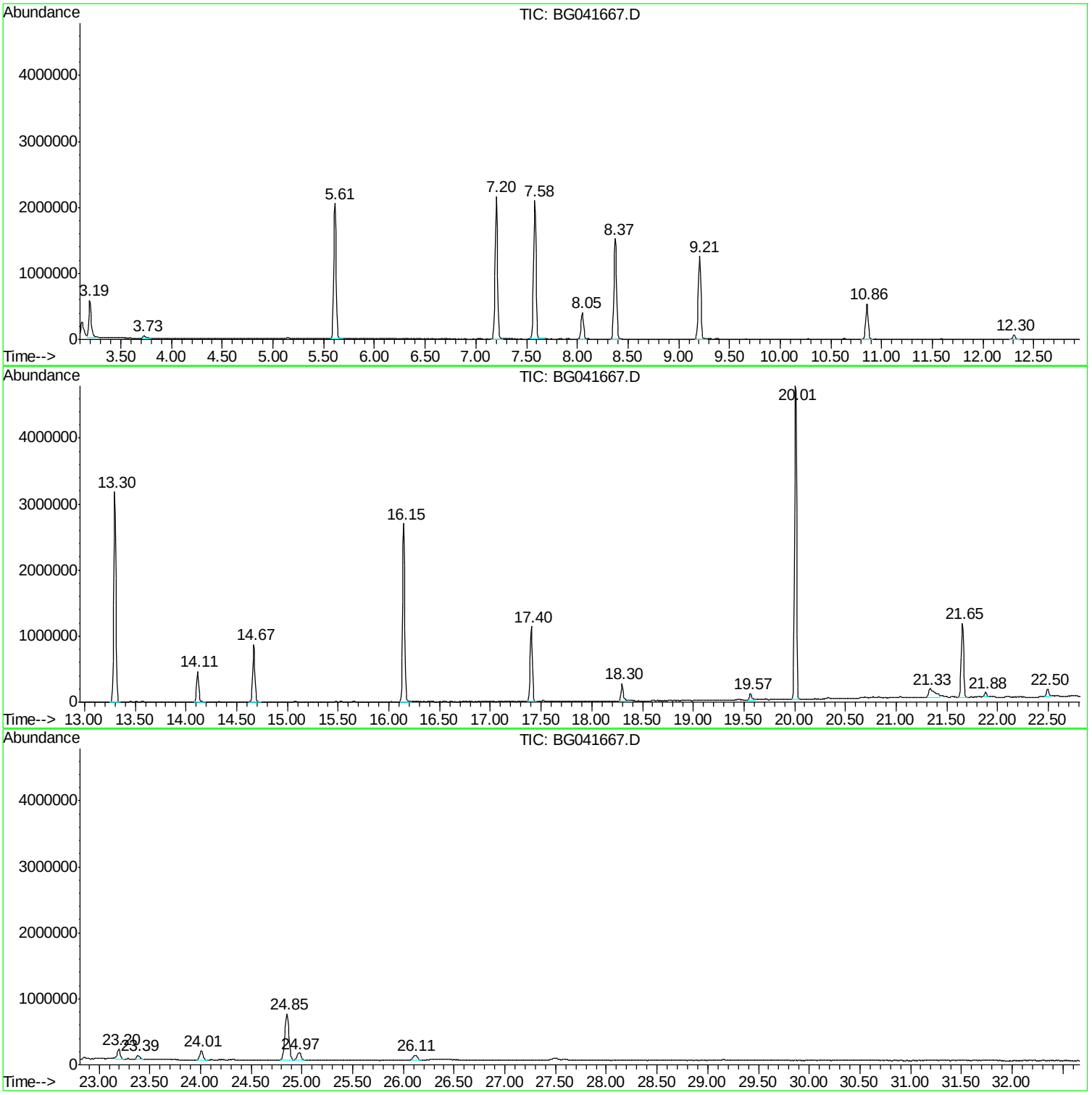
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

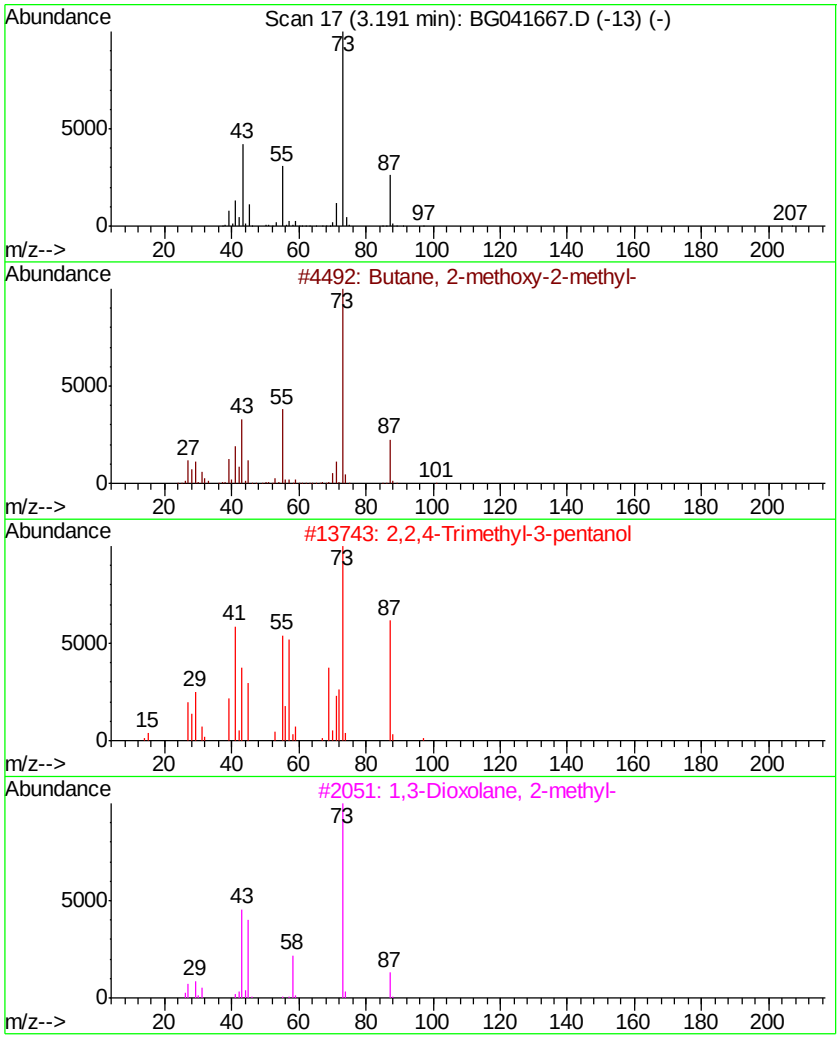
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

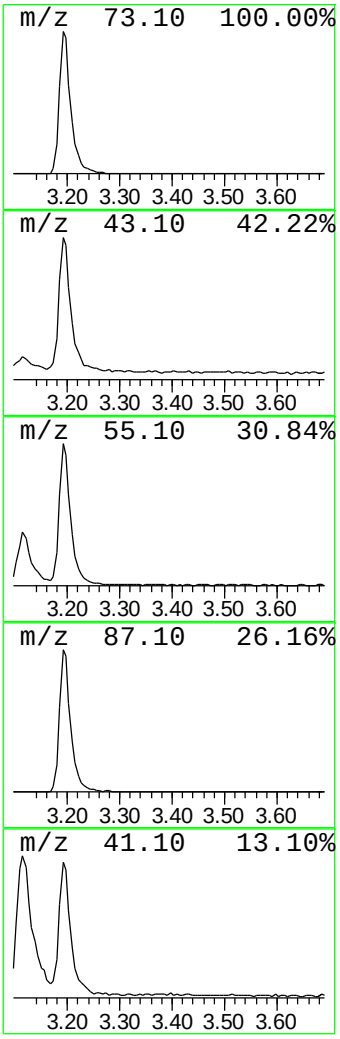
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	25.75 ng	873272	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

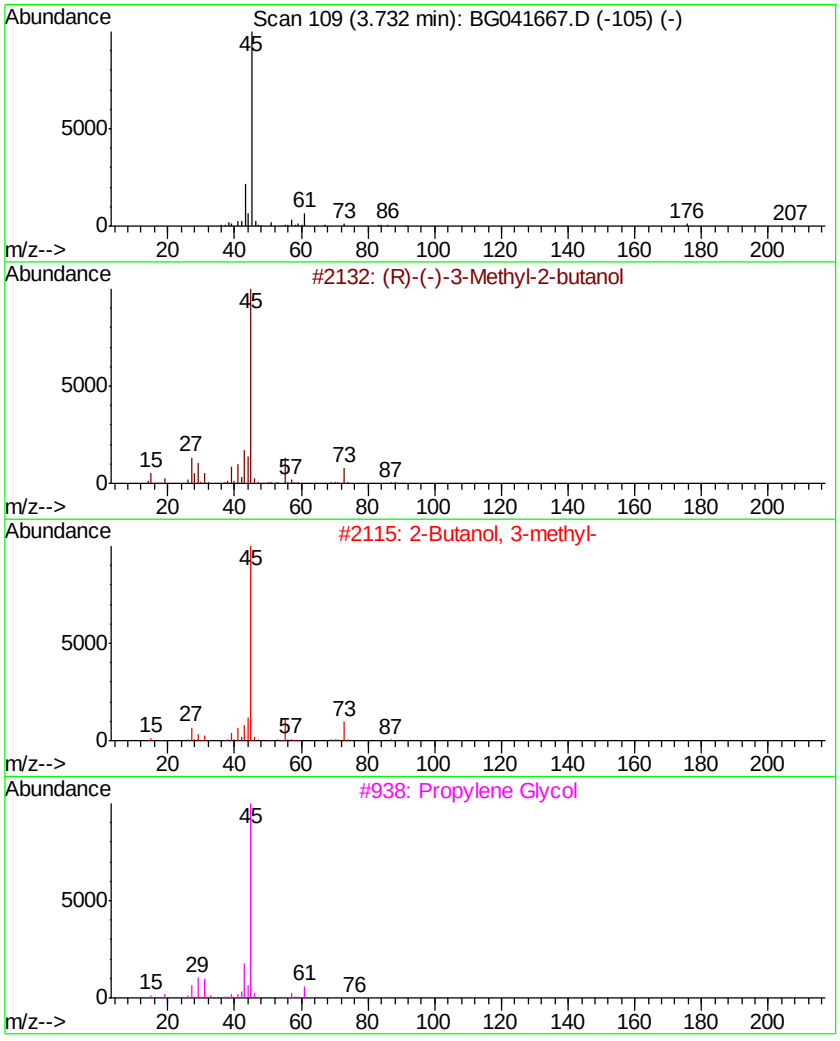
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

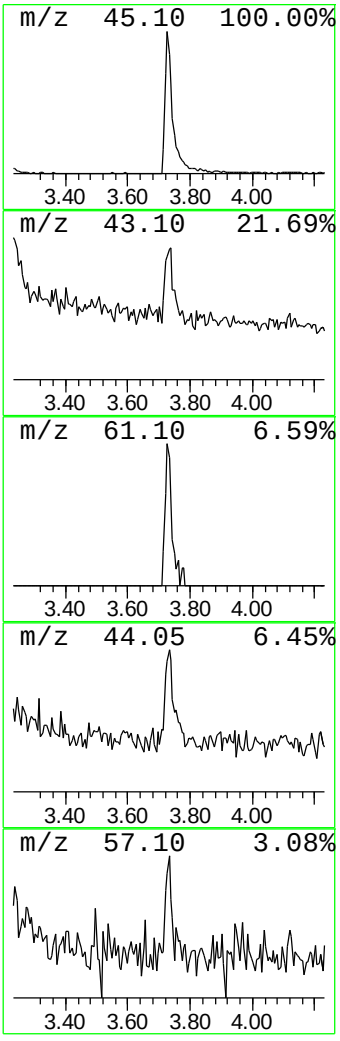
****

Peak Number 2 (R)-(-)-3-Methyl-2-butanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	2.04 ng	69283	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	64
2	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	50
3	Propylene Glycol	76	C3H8O2	000057-55-6	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
5	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	39





Library Search Compound Report

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Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

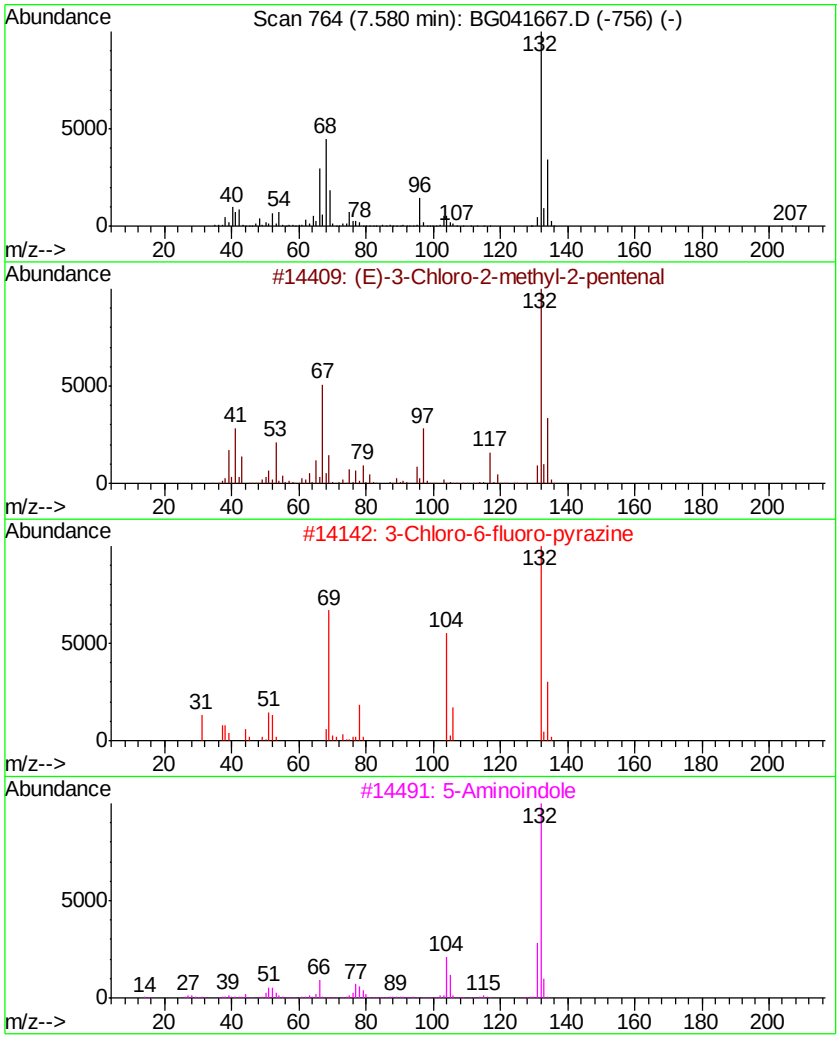
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

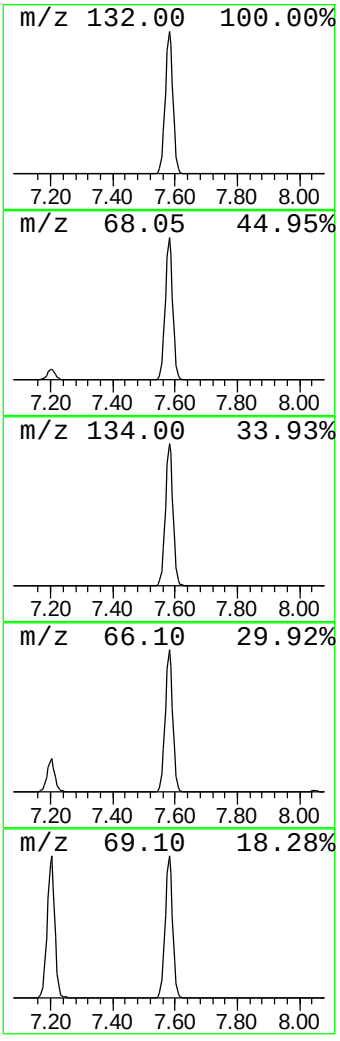
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	105.75 ng	3585680	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
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\BG071619\
Data File : BG041667.D
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Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

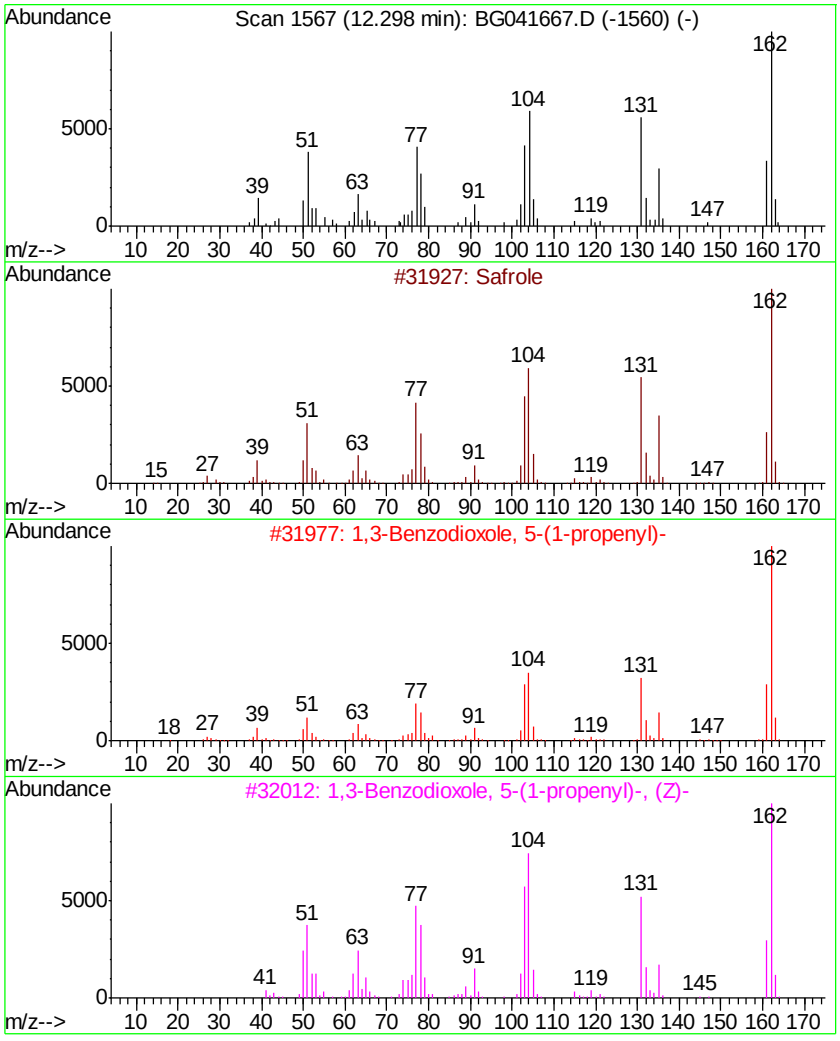
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

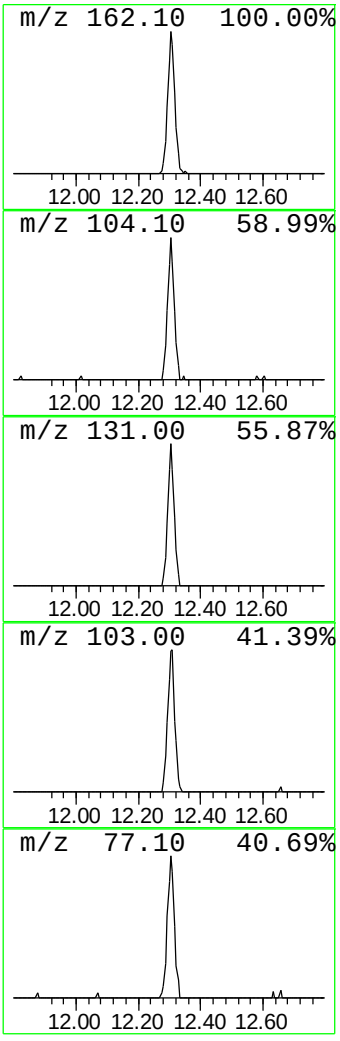
****

Peak Number 5 Safrole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.27 ng	112815	Naphthalene-d8	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	96
3	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	94
4	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	94
5	1H-Isoindole-1,3(2H)-dione, 2-am...	162	C8H6N2O2	001875-48-5	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
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Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

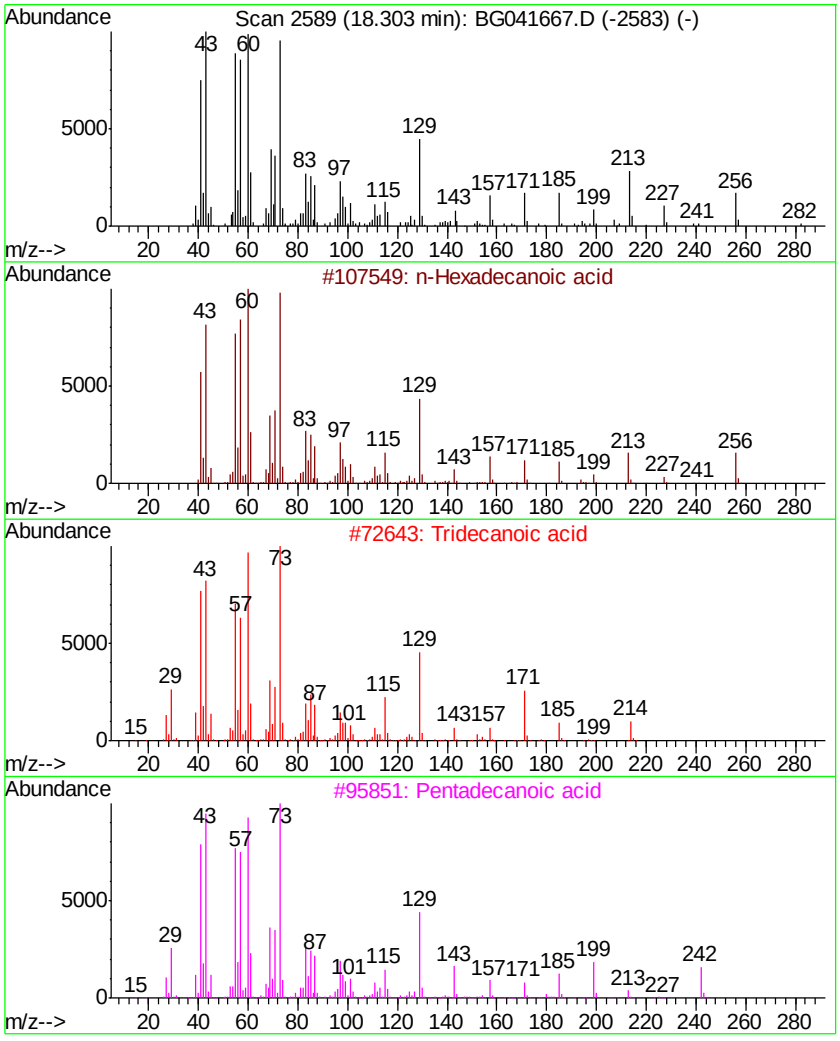
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

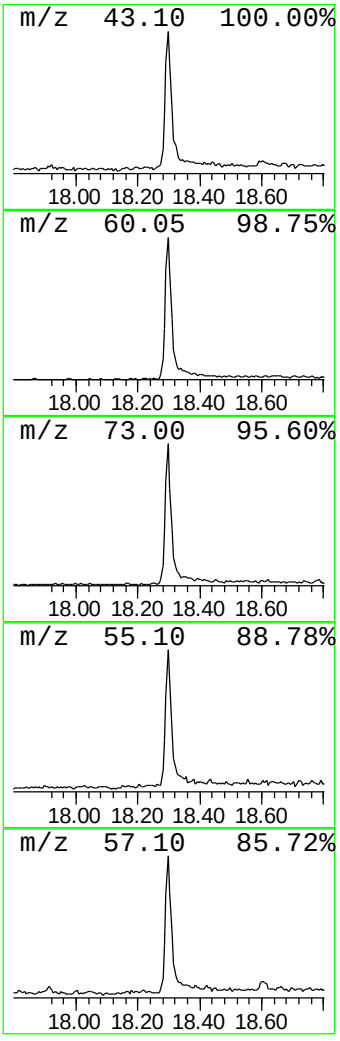
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	4.77 ng	410131	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
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Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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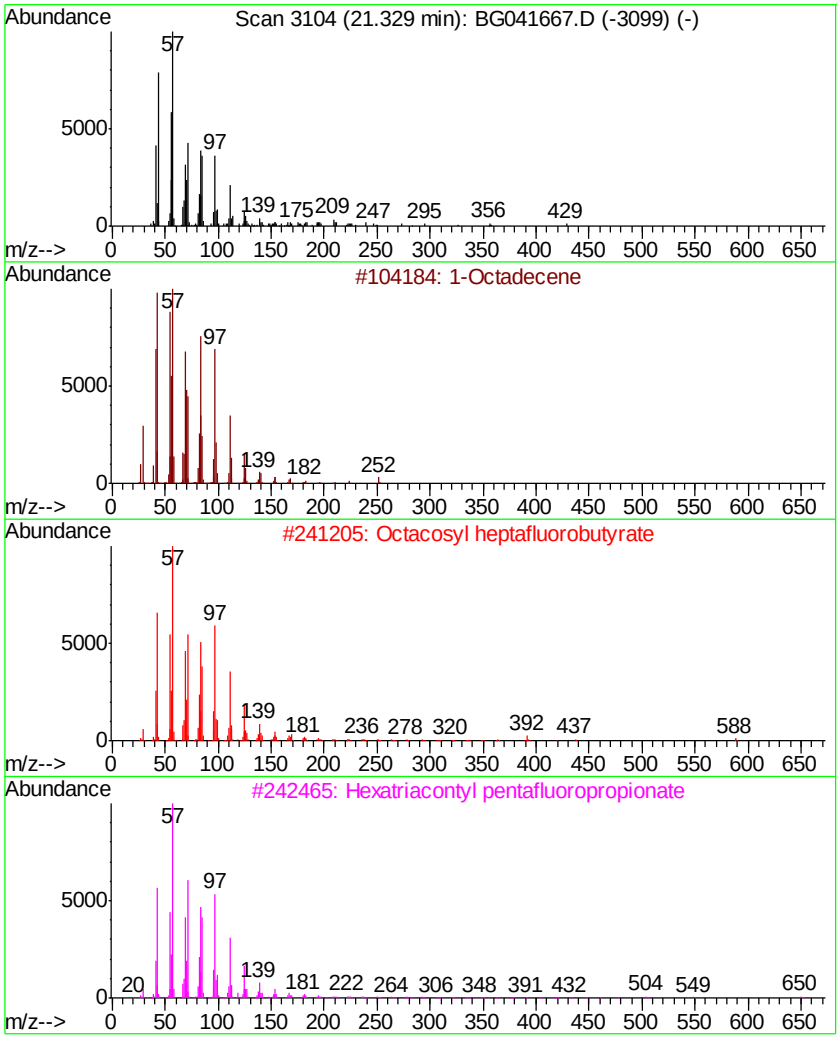
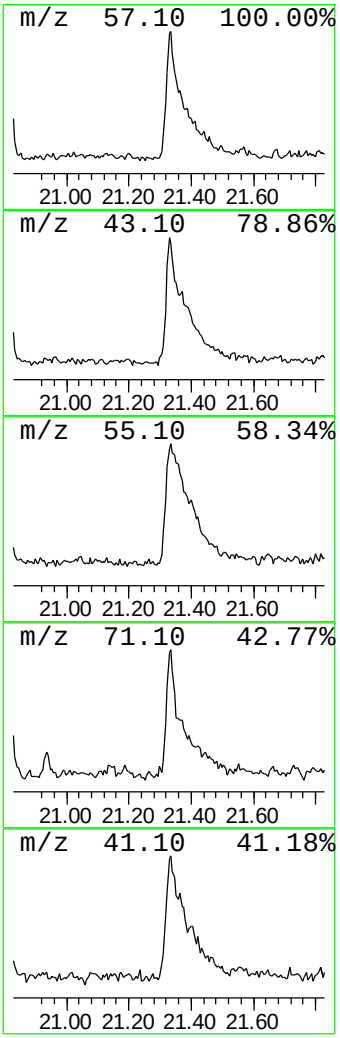
****

Peak Number 7 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	6.27 ng	586787	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
3	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
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Sample : K3826-03
Misc :
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Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

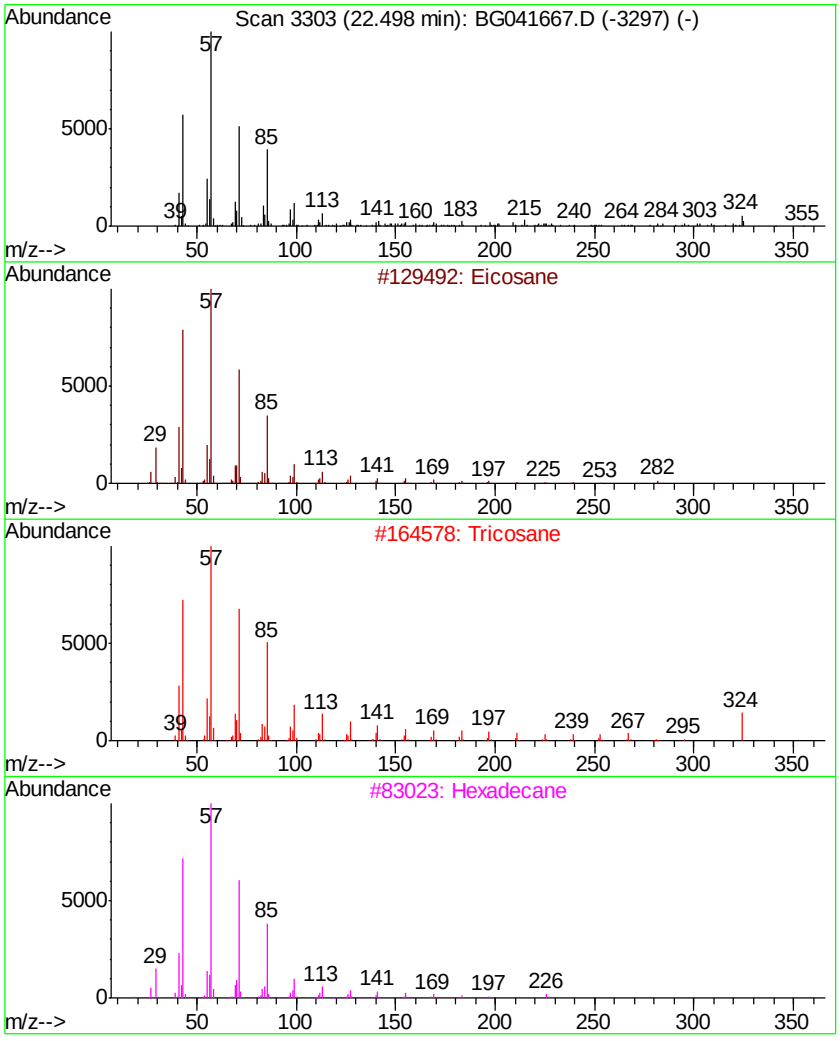
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

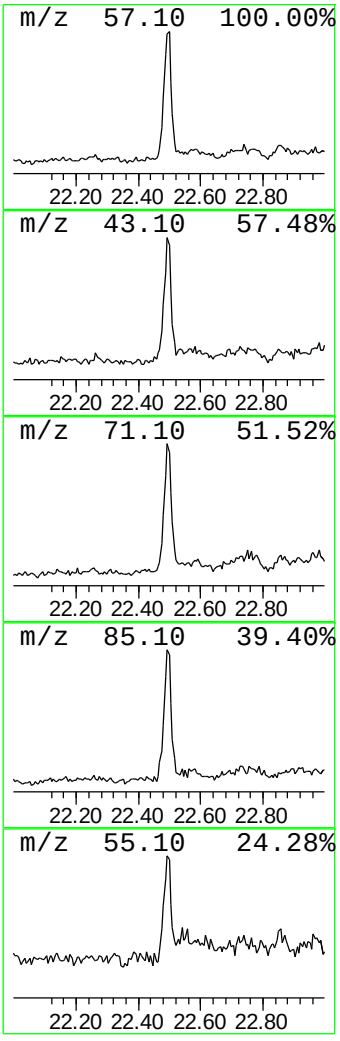
****

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	2.19 ng	205235	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Tricosane	324	C23H48	000638-67-5	93
3	Hexadecane	226	C16H34	000544-76-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

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TIC Library : C:\Database\NIST11.L
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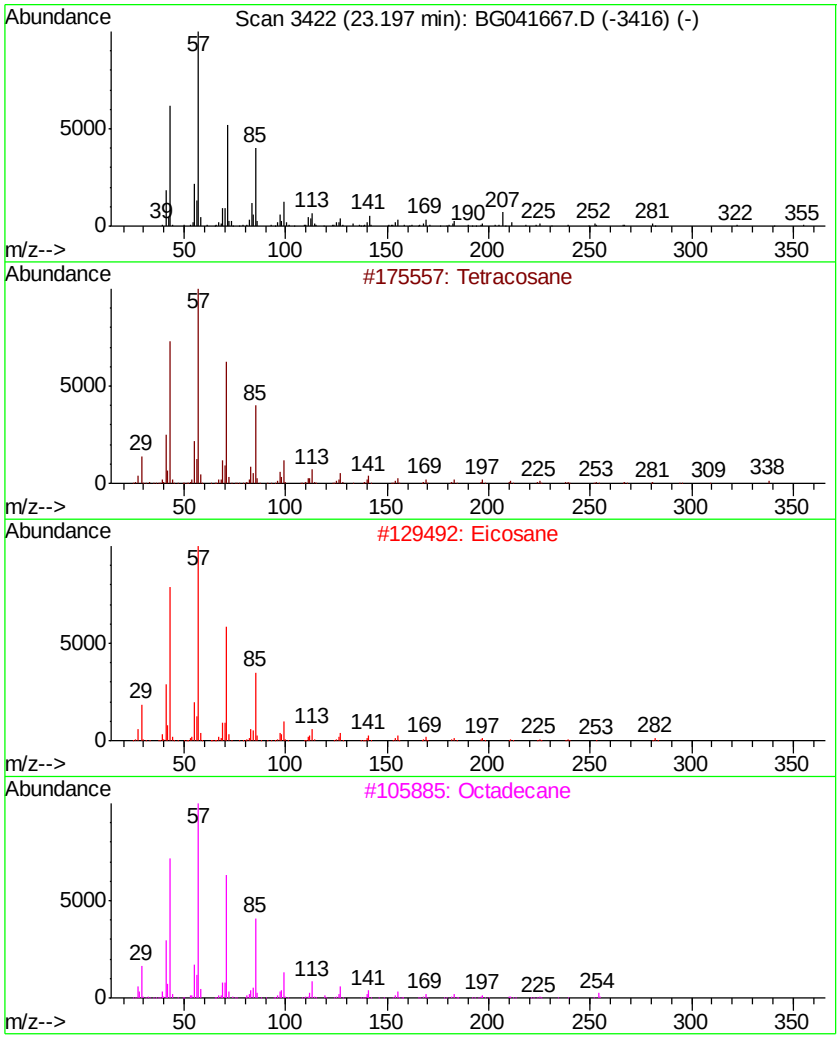
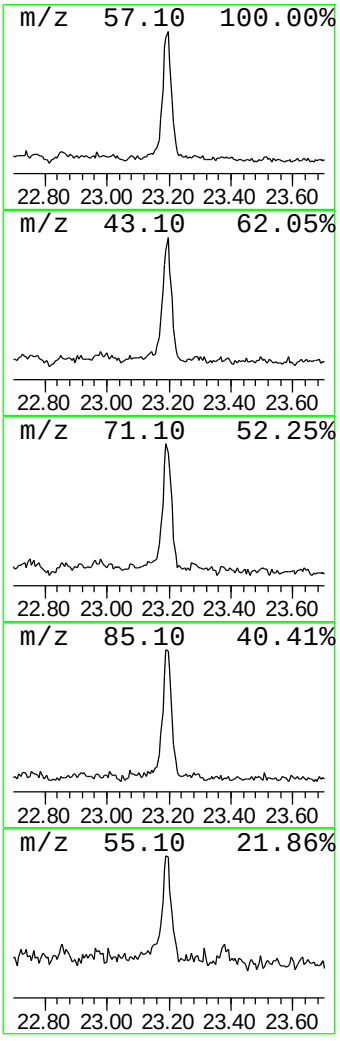
Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	3.29 ng	307343	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Eicosane	282	C20H42	000112-95-8	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	86
5	Tetradecane	198	C14H30	000629-59-4	86





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Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
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Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

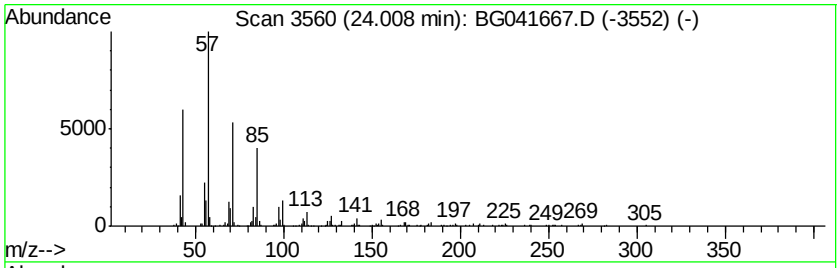
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

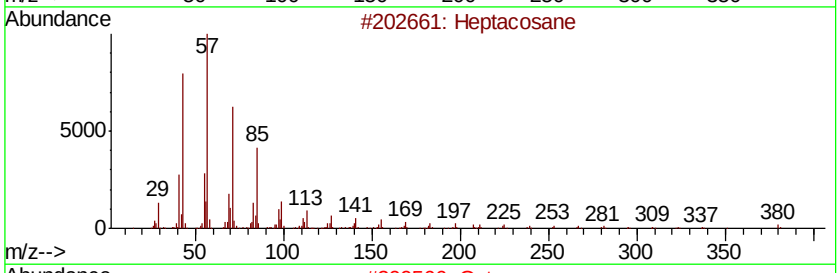
****

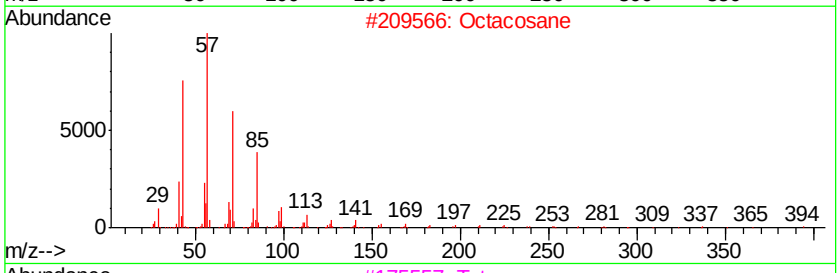
Peak Number 10 Heptacosane Concentration Rank 6

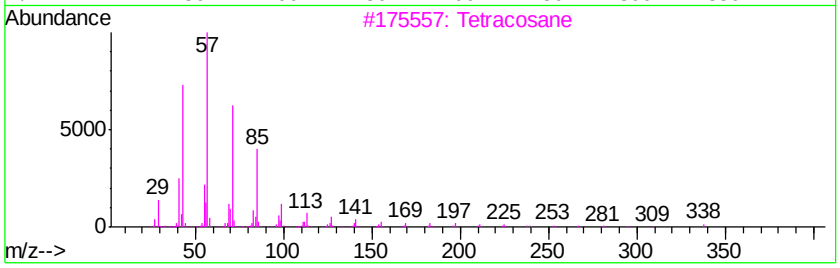
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.01	3.56 ng	344789	Perylene-d12	24.85

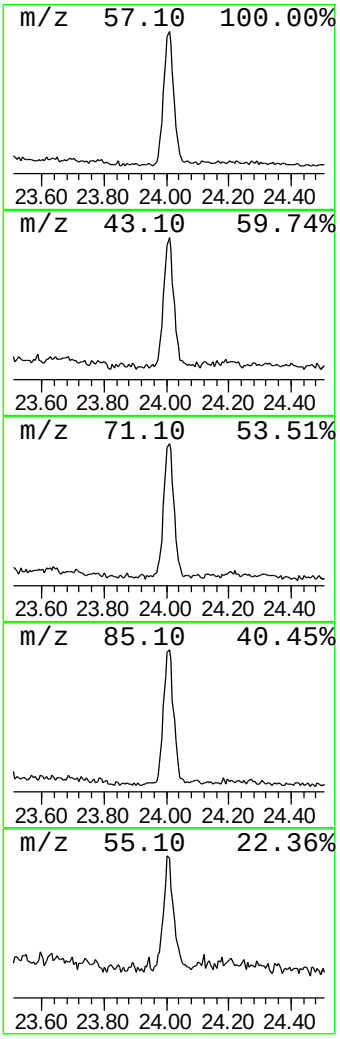
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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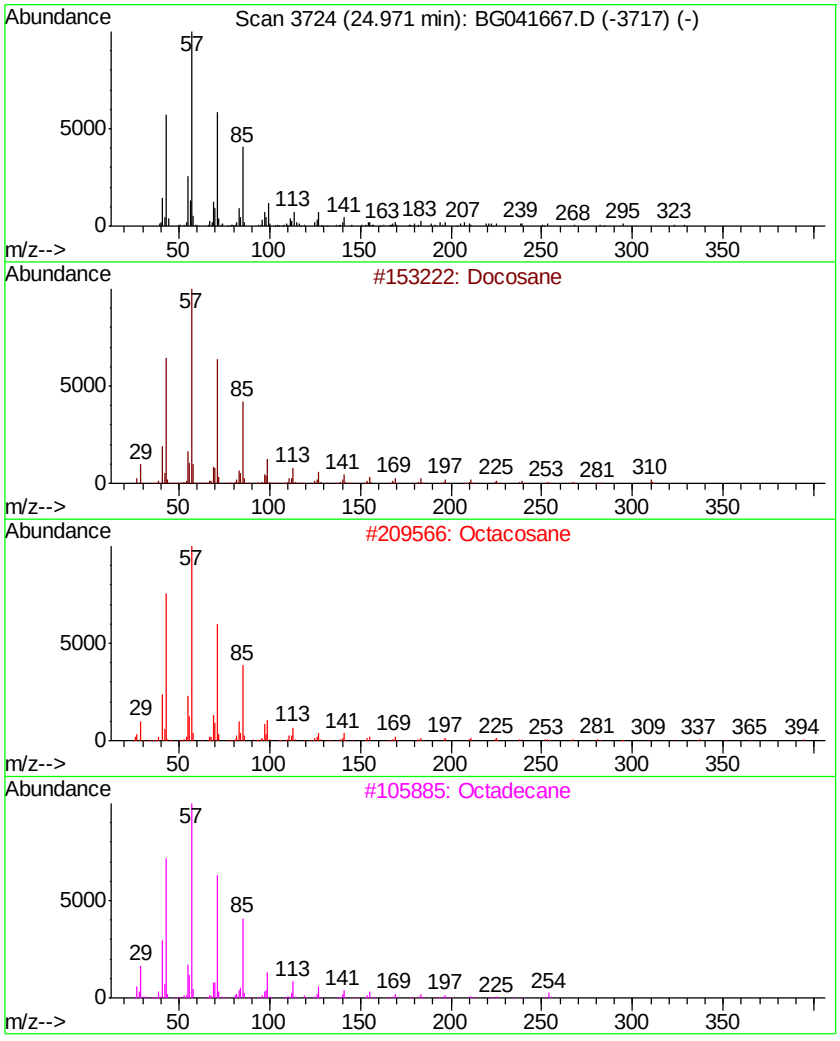
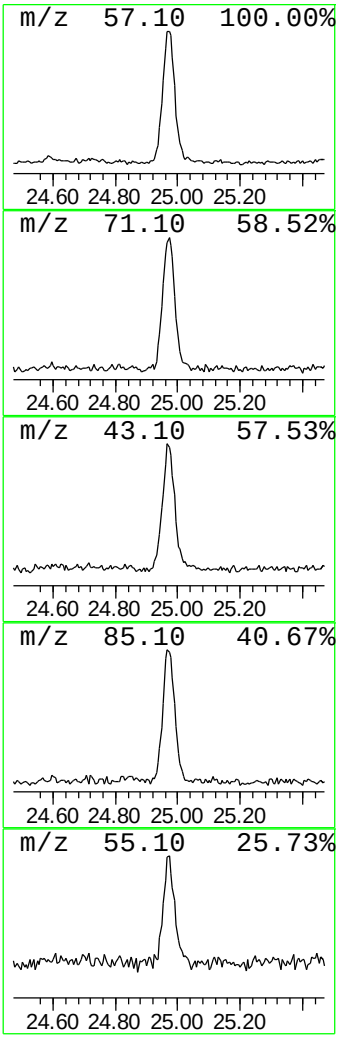
Peak Number 11 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	2.96 ng	286827	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Eicosane	282	C20H42	000112-95-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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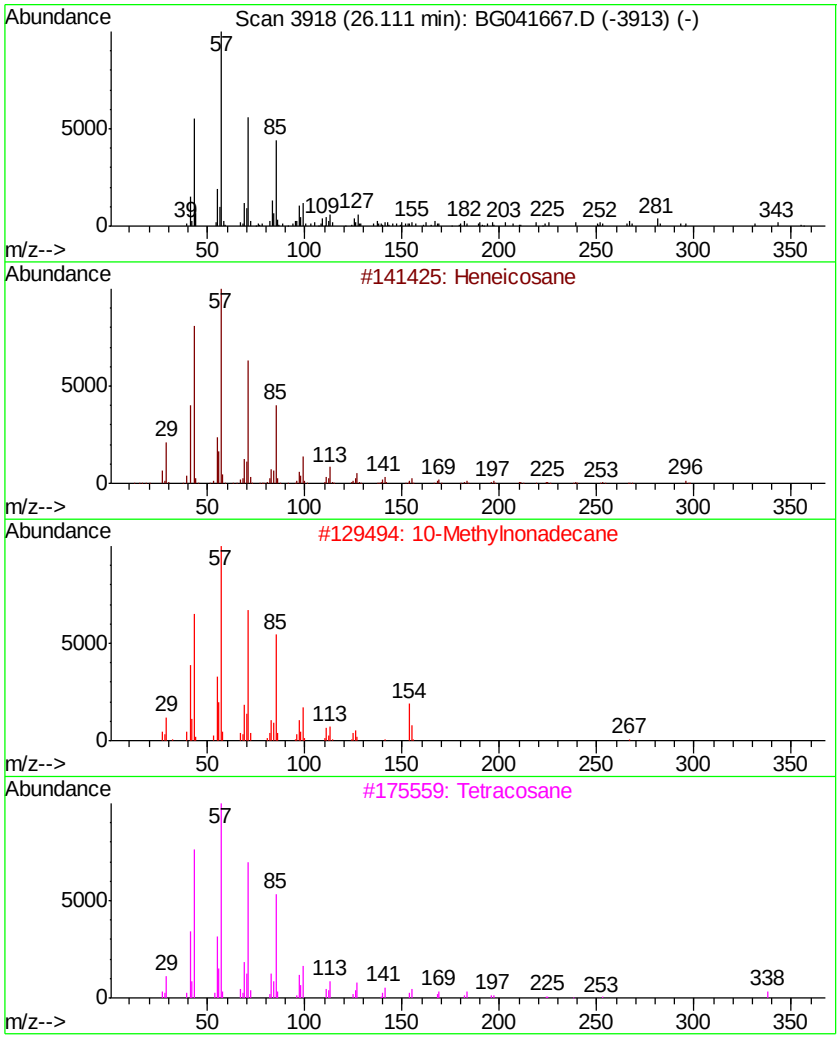
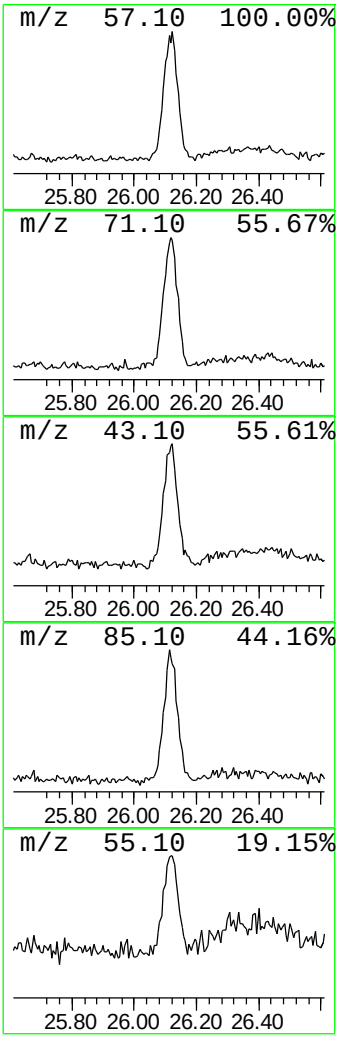
Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.11	2.37 ng	229483	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	10-Methylnonadecane	282	C20H42	056862-62-5	72
3	Tetracosane	338	C24H50	000646-31-1	64
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
5	Nonadecane	268	C19H40	000629-92-5	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071619\
Data File : BG041667.D
Acq On : 16 Jul 2019 14:25
Operator : HP/JU
Sample : K3826-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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	25.8	ng	873272	1	8.05	678154	20.0
(R)-(-)-3-Methyl-...	3.73	2.0	ng	69283	1	8.05	678154	20.0
unknown7.58	7.58	105.8	ng	3585680	1	8.05	678154	20.0
Safrole	12.30	2.3	ng	112815	2	10.86	992306	20.0
n-Hexadecanoic acid	18.30	4.8	ng	410131	4	17.40	1720900	20.0
1-Octadecene	21.33	6.3	ng	586787	5	21.65	1870470	20.0
Eicosane	22.50	2.2	ng	205235	5	21.65	1870470	20.0
Tetracosane	23.20	3.3	ng	307343	5	21.65	1870470	20.0
Heptacosane	24.01	3.6	ng	344789	6	24.85	1935600	20.0
Docosane	24.97	3.0	ng	286827	6	24.85	1935600	20.0
Heneicosane	26.11	2.4	ng	229483	6	24.85	1935600	20.0