LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
Data File : BG041731.D
Acq On : 19 Jul 2019 12:29
Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-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-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	3.193	13	18	30	rVB	294092	524789	9.78%	1.521%
2	5.608	422	429	440	rBV	1362607	2180086	40.62%	6.318%
3	7.200	690	700	719	rBV	1365104	2444216	45.54%	7.083%
4	7.576	755	764	771	rBV	1400261	2366032	44.09%	6.857%
5	8.046	837	844	852	rBV	367617	624857	11.64%	1.811%
6	8.369	891	899	911	rVB	1060968	1830972	34.12%	5.306%
7	9.198	1032	1040	1054	rBV	817086	1451663	27.05%	4.207%
8	10.849	1313	1321	1330	rBV	472791	857899	15.99%	2.486%
9	13.293	1730	1737	1746	rBV	2097587	3252692	60.61%	9.426%
10	14.110	1870	1876	1884	rBV	245131	346357	6.45%	1.004%
11	14.662	1963	1970	1978	rBV2	721469	1175073	21.89%	3.405%
12	16.142	2215	2222	2234	rBV	1778781	2754022	51.32%	7.981%
13	17.400	2429	2436	2449	rBV2	997691	1576973	29.38%	4.570%
14	18.287	2580	2587	2596	rBV3	61399	123418	2.30%	0.358%
15	19.439	2777	2783	2791	rBV3	27298	58155	1.08%	0.169%
16	19.803	2840	2845	2852	rVB2	29021	59044	1.10%	0.171%
17	20.003	2873	2879	2892	rVB	3998356	5366878	100.00%	15.553%
18	21.307	3096	3101	3116	rBV2	235057	537245	10.01%	1.557%
19	21.648	3152	3159	3168	rBV	1250233	2020825	37.65%	5.856%
20	21.865	3192	3196	3199	rBV2	123379	202962	3.78%	0.588%
21	21.971	3207	3214	3218	rBV4	171835	488297	9.10%	1.415%
22	22.153	3239	3245	3246	rBV4	291766	576009	10.73%	1.669%
23	23.164	3413	3417	3427	rVB	213144	440326	8.20%	1.276%
24	23.980	3548	3556	3564	rBV	185494	420690	7.84%	1.219%
25	24.838	3692	3702	3711	rBV2	736601	2092029	38.98%	6.063%
26	24.926	3712	3717	3729	rVB3	165662	402633	7.50%	1.167%
27	26.066	3904	3911	3924	rVB2	108705	332226	6.19%	0.963%

Sum of corrected areas: 34506368

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
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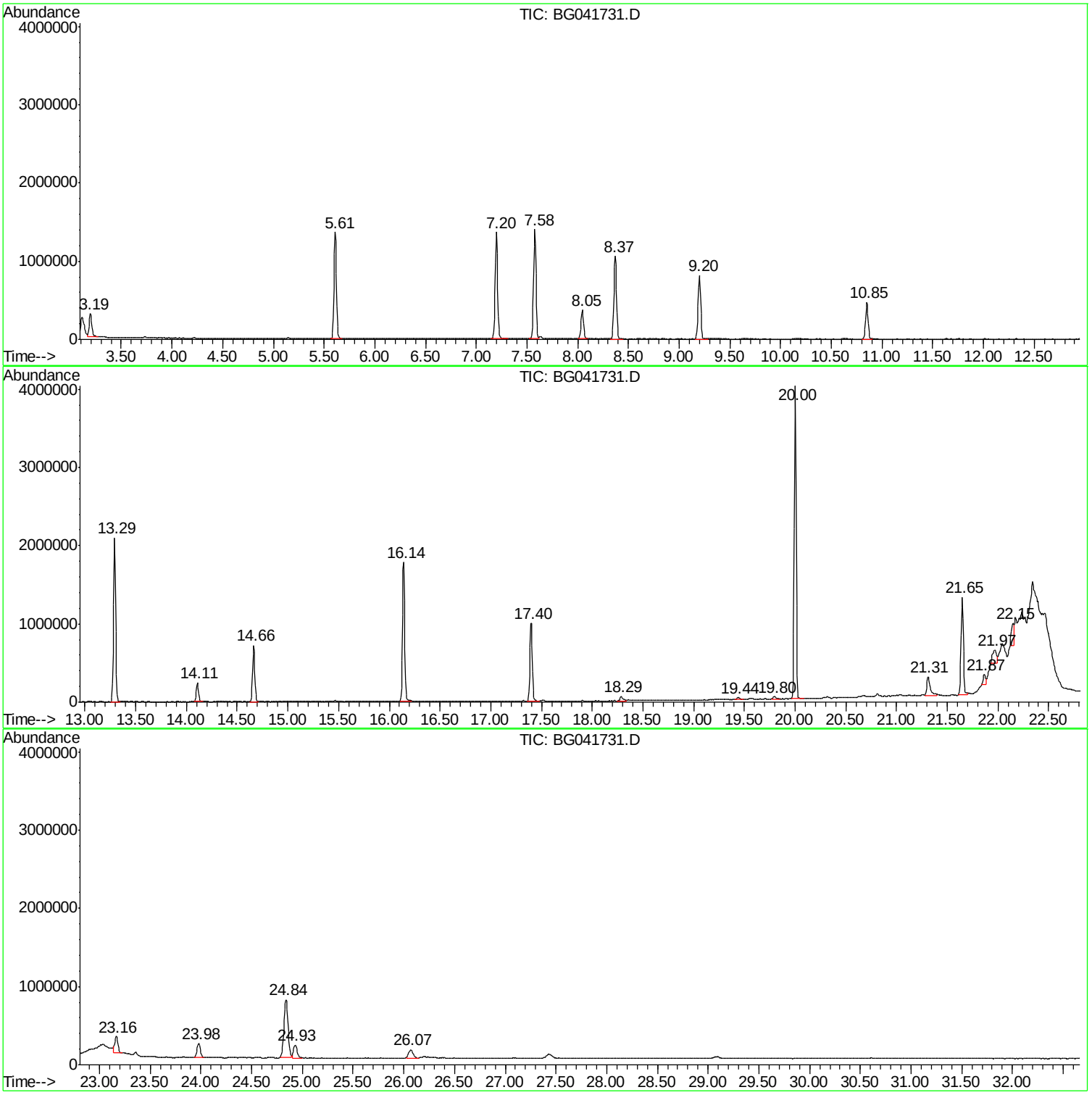
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

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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ClientSampleId : TP-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

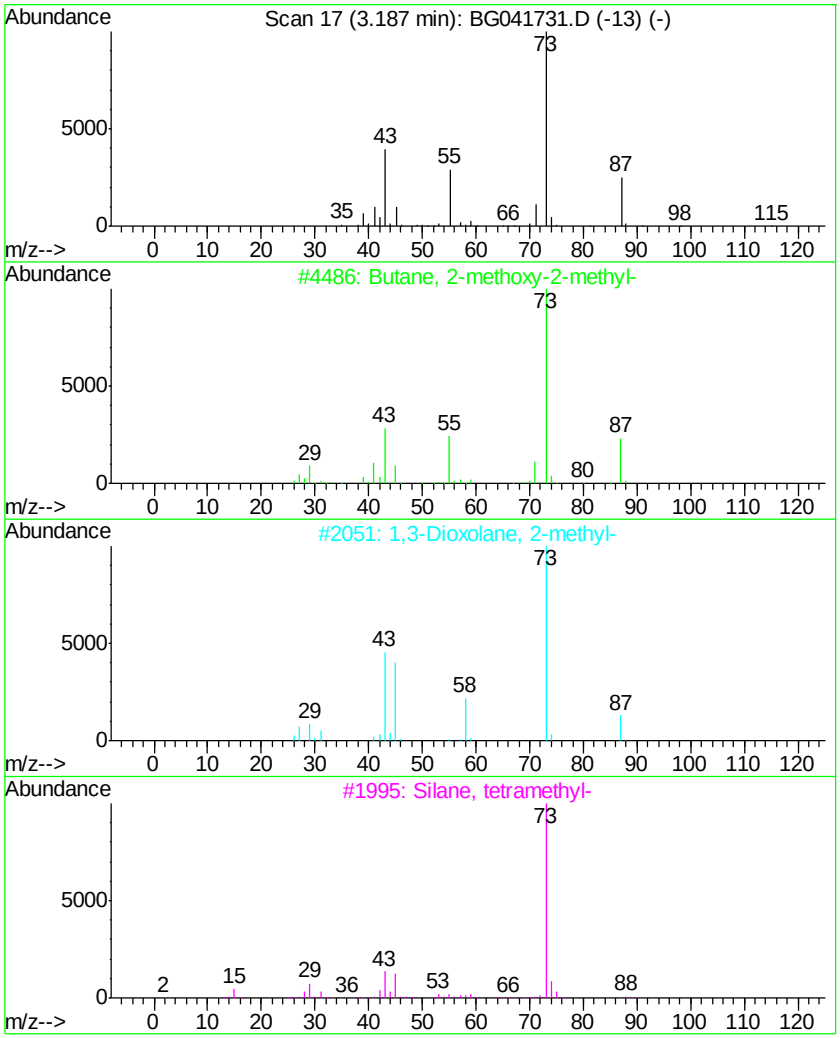
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

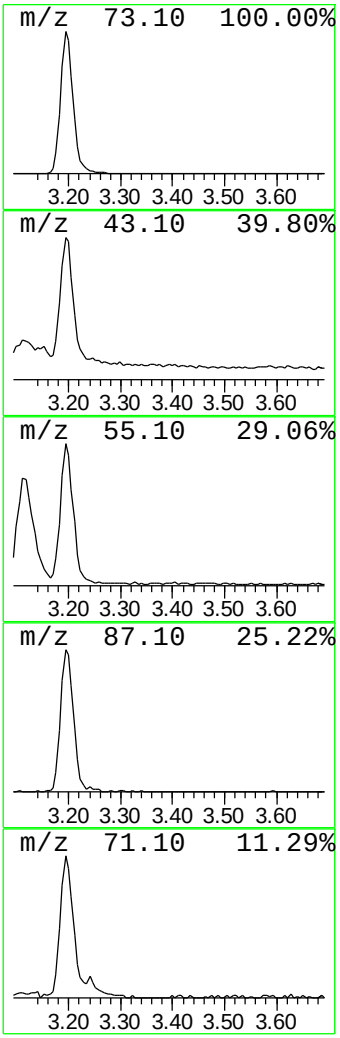
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	16.80 ng	524789	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	74
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Operator : HP/JU
Sample : K3868-11
Misc :
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Instrument : BNA_G
ClientSampleId : TP-4

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

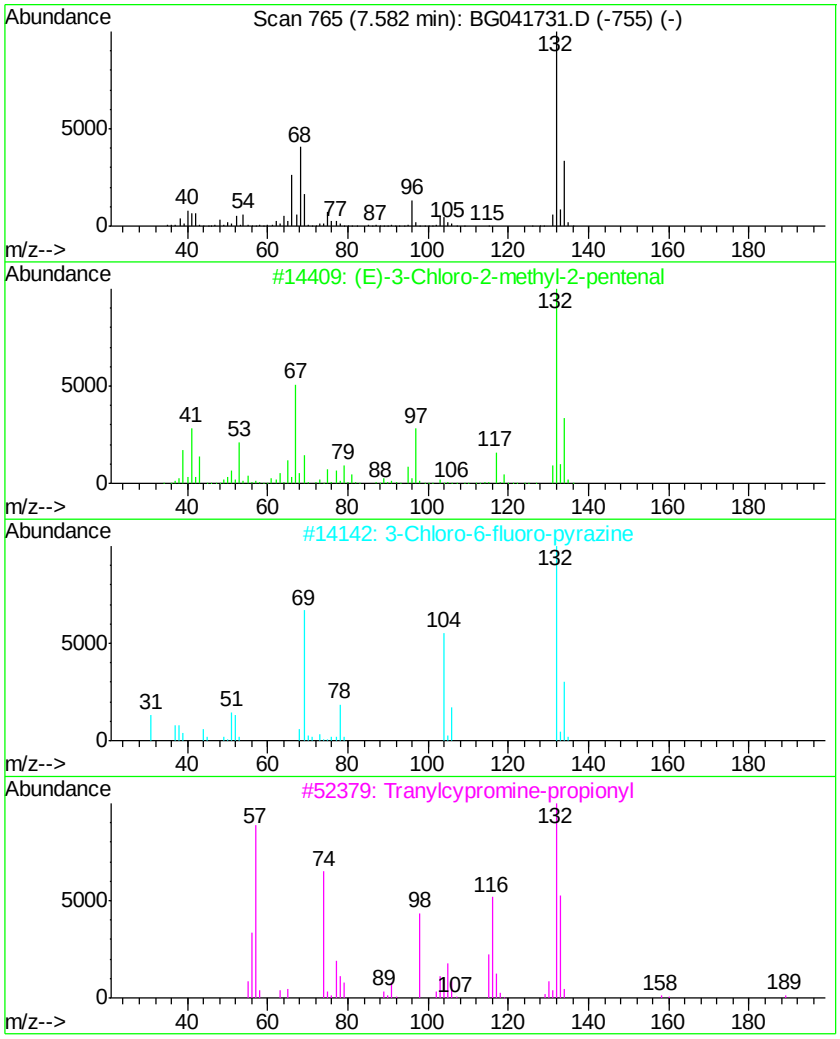
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

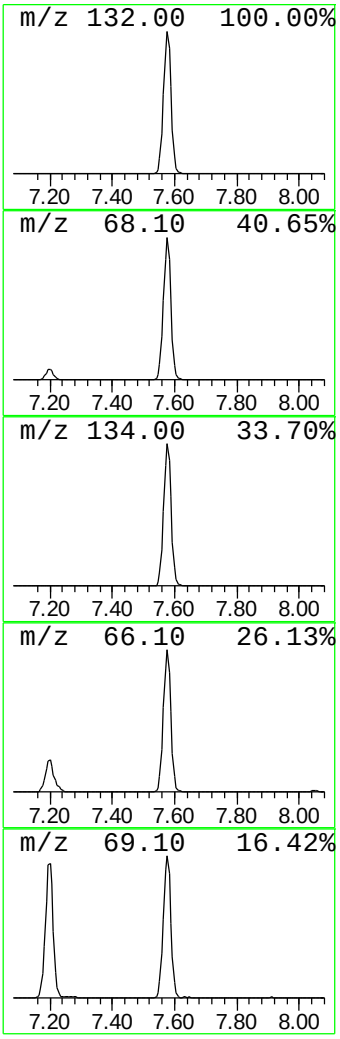
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	75.73 ng	2366030	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	30
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BG041731.D
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Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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

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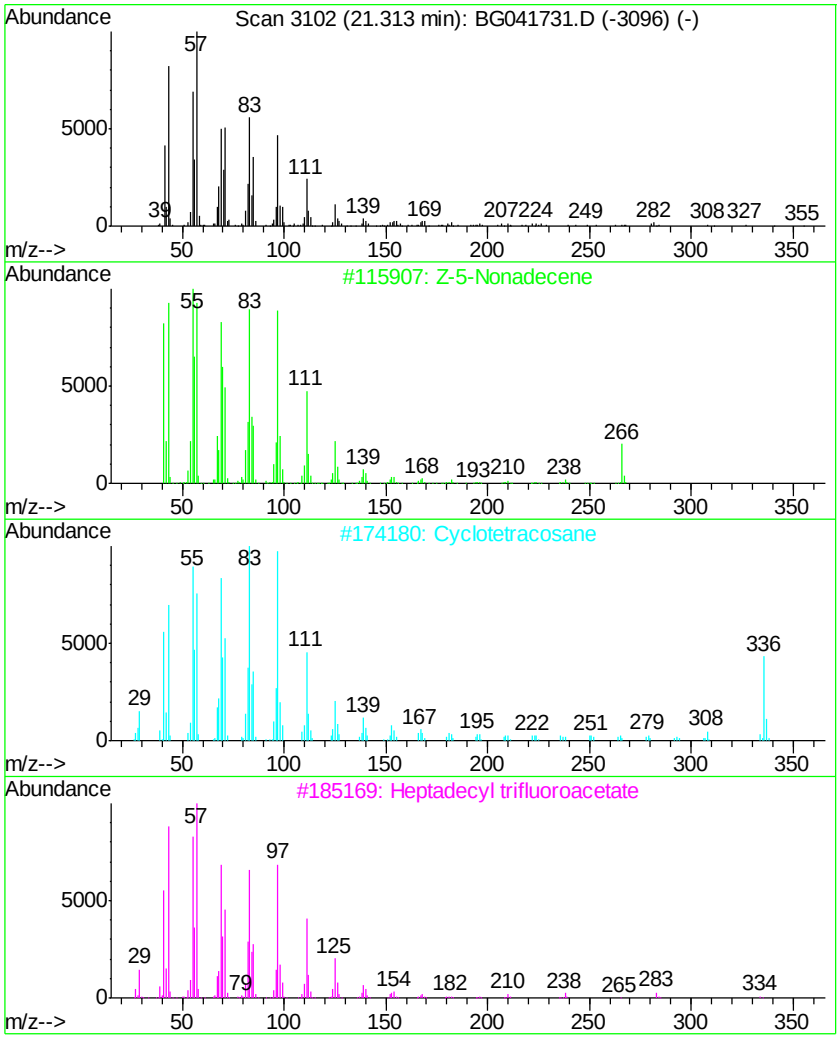
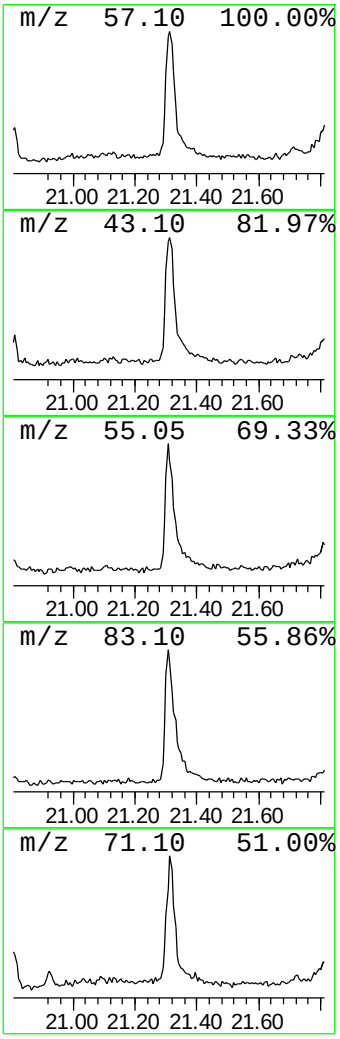
****

Peak Number 4 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.32 ng	537245	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	95
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Nonadecene	266	C19H38	018435-45-5	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
Data File : BG041731.D
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Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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

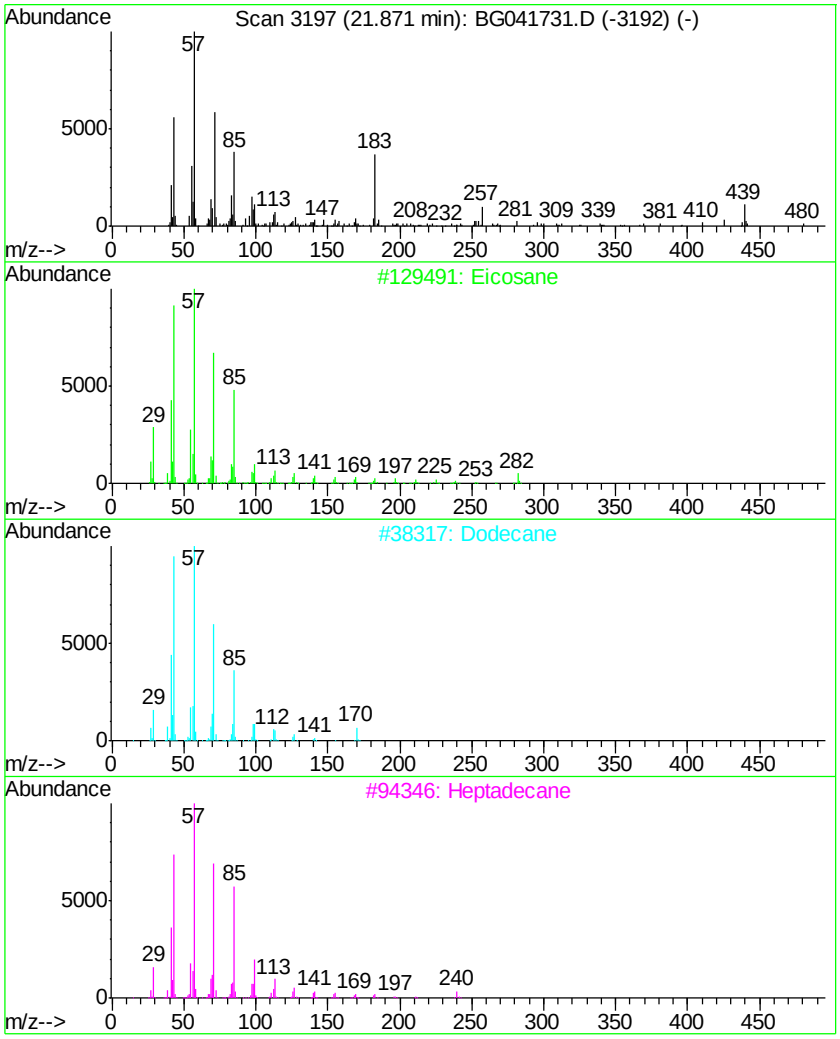
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

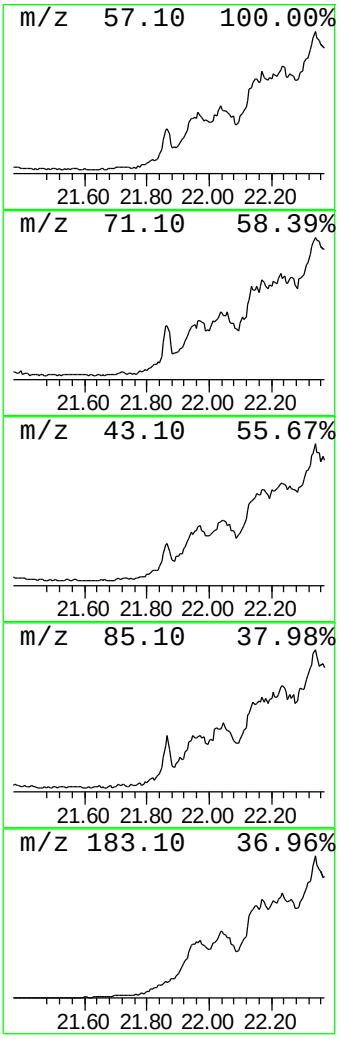
****

Peak Number 5 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	2.01 ng	202962	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	70
2	Dodecane	170	C12H26	000112-40-3	70
3	Heptadecane	240	C17H36	000629-78-7	68
4	Tetracosane	338	C24H50	000646-31-1	64
5	Pentadecane	212	C15H32	000629-62-9	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
Data File : BG041731.D
Acq On : 19 Jul 2019 12:29
Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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

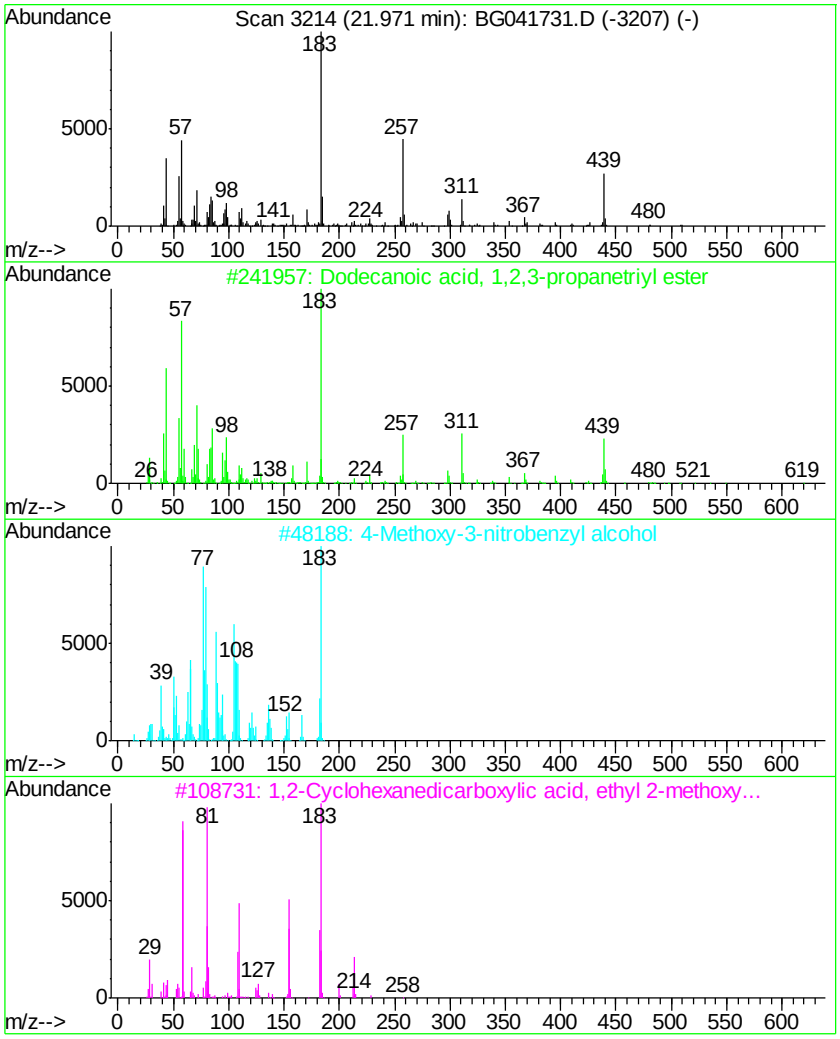
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

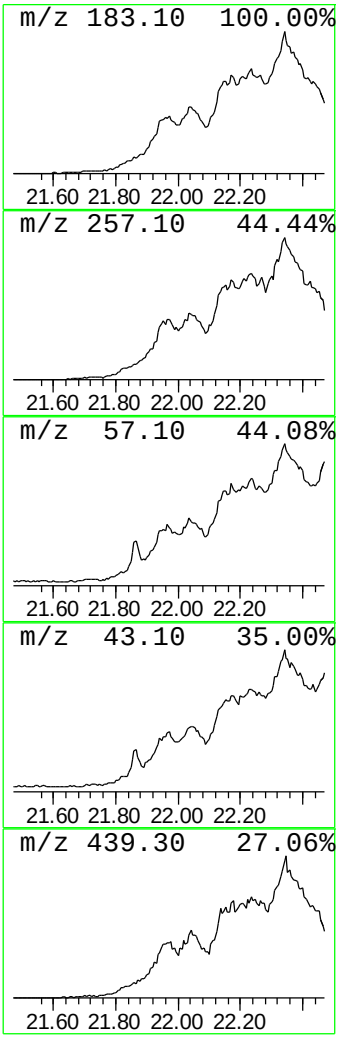
****

Peak Number 6 unknown21.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	4.83 ng	488297	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 1,2,3-propanetr...	639	C39H74O6	000538-24-9	46
2	4-Methoxy-3-nitrobenzyl alcohol	183	C8H9NO4	041870-24-0	43
3	1,2-Cyclohexanedicarboxylic acid...	258	C13H22O5	1000340-02-3	43
4	Lauric anhydride	382	C24H46O3	000645-66-9	38
5	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
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Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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

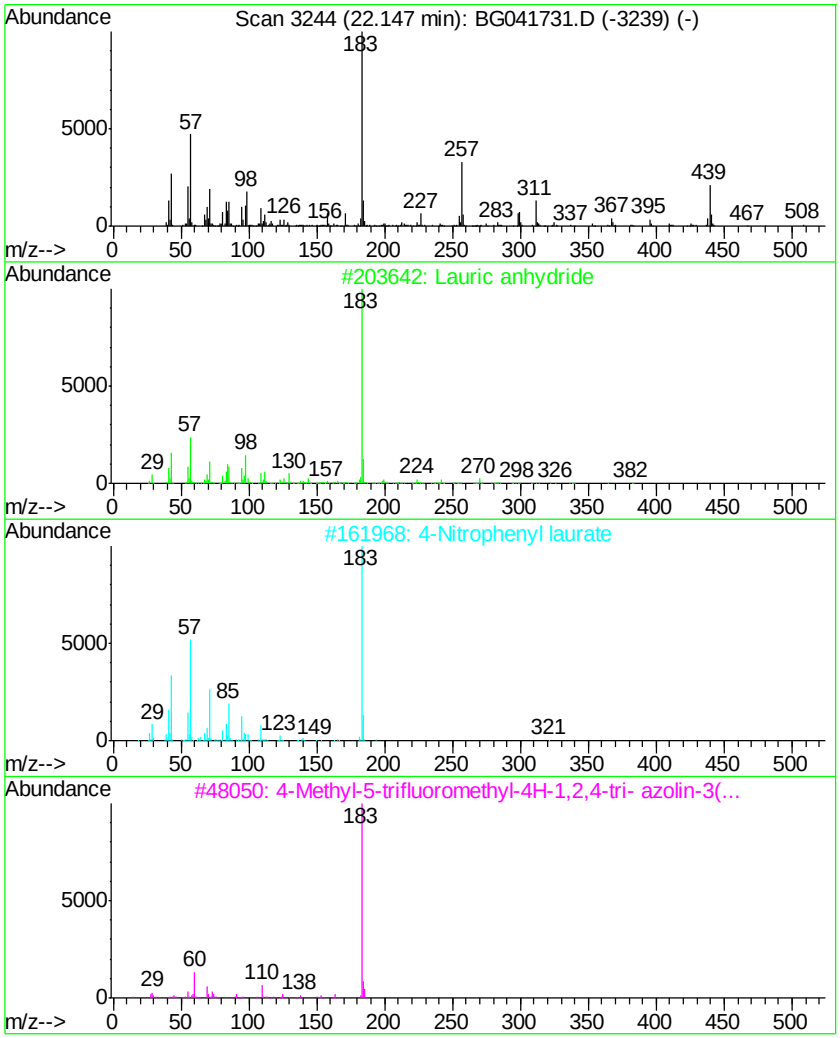
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

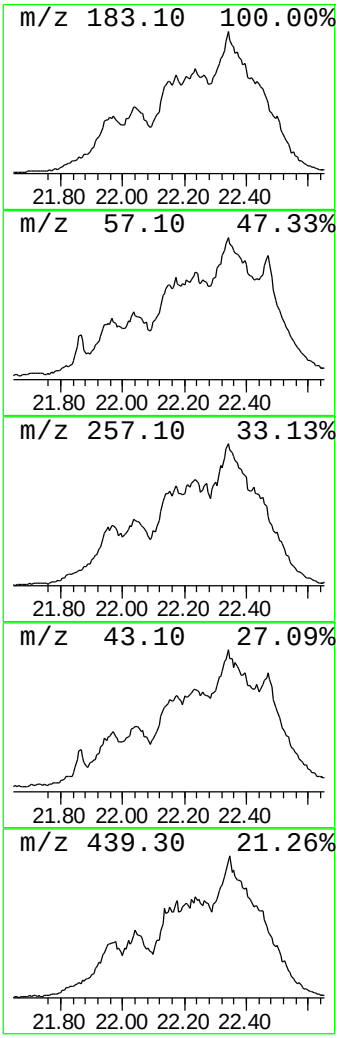
****

Peak Number 7 Lauric anhydride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.15	5.70 ng	576009	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauric anhydride	382	C24H46O3	000645-66-9	55
2	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	49
3	4-Methyl-5-trifluoromethyl-4H-1,...	183	C4H4F3N3S	030682-81-6	46
4	4-Dibenzofuranamine	183	C12H9NO	050548-43-1	46
5	Fumaric acid, 3,5-difluorophenyl...	312	C16H18F2O4	1000339-37-2	43





Library Search Compound Report

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Data File : BG041731.D
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Misc :
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Instrument : BNA_G
ClientSampleId : TP-4

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

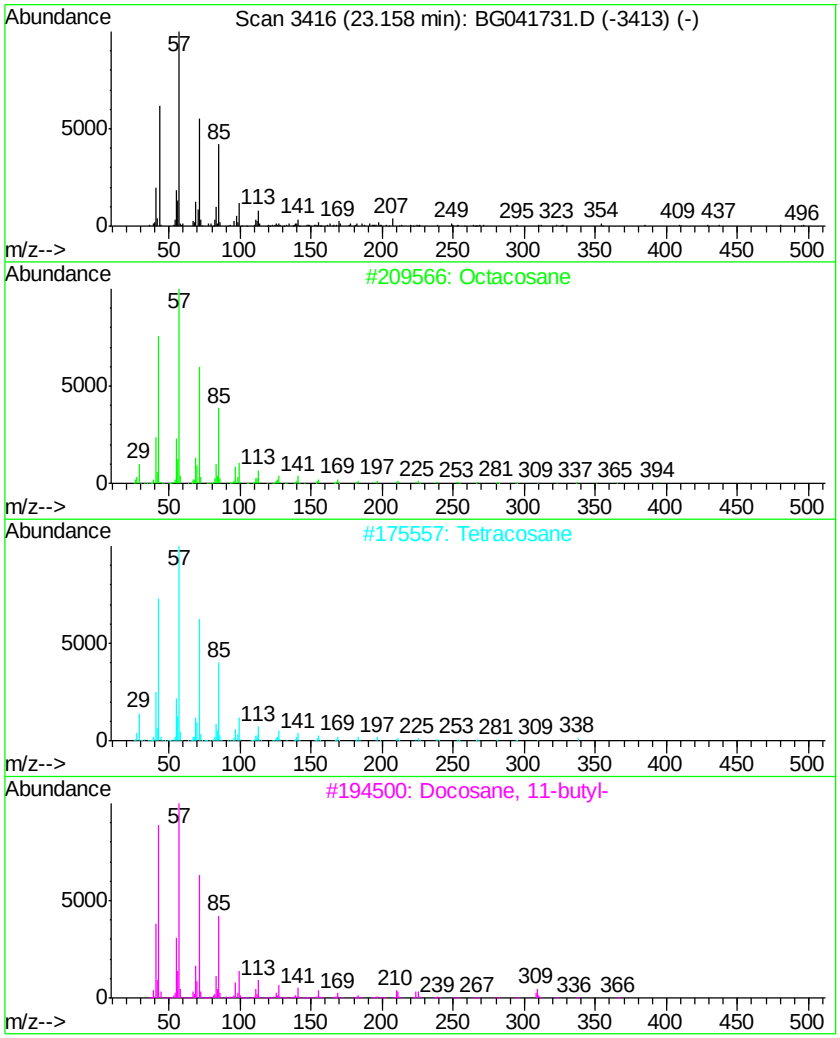
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

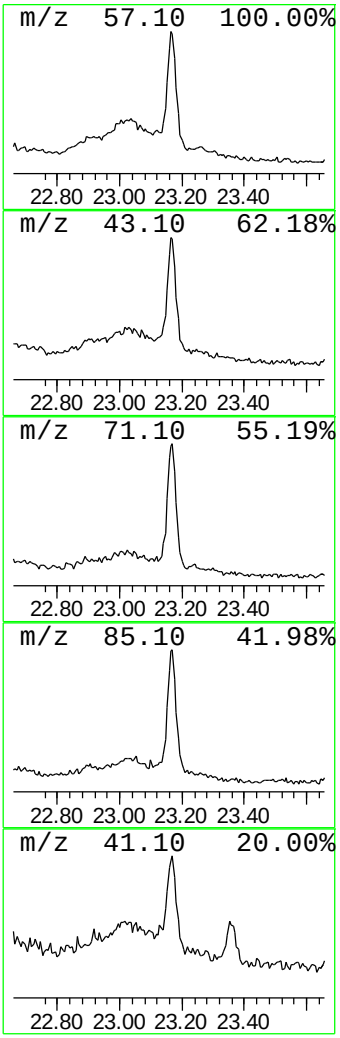
****

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	4.36 ng	440326	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86





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Instrument : BNA_G
ClientSampleId : TP-4

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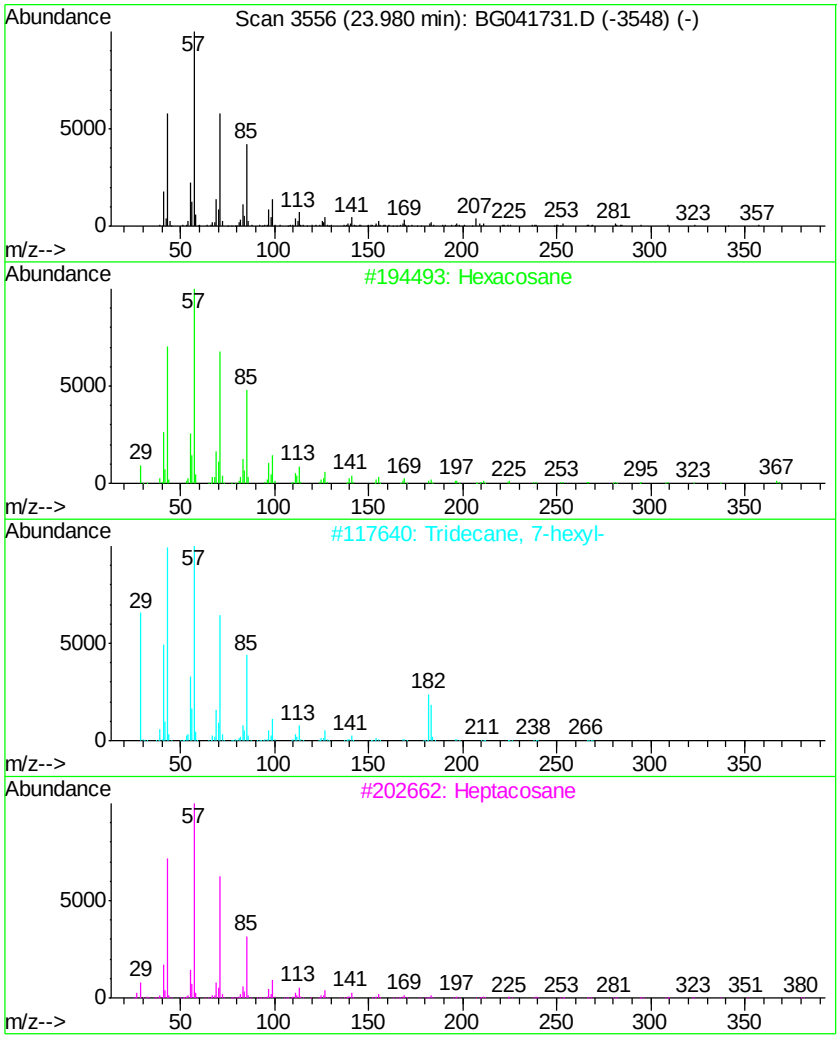
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

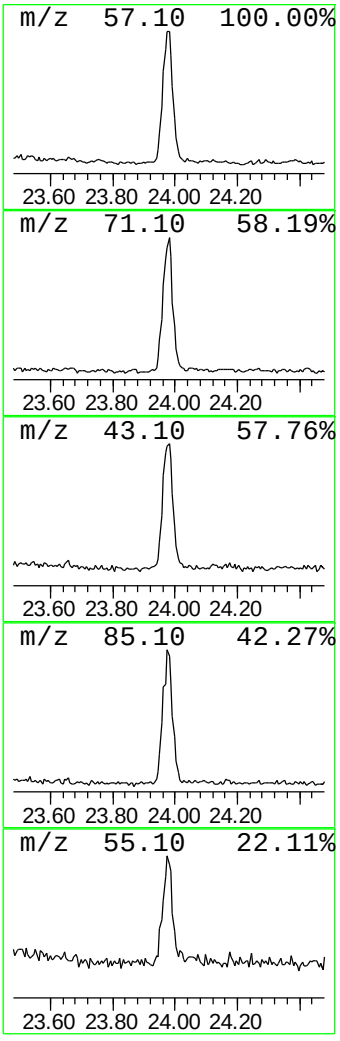
****

Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	4.02 ng	420690	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Eicosane	282	C20H42	000112-95-8	90





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-4

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

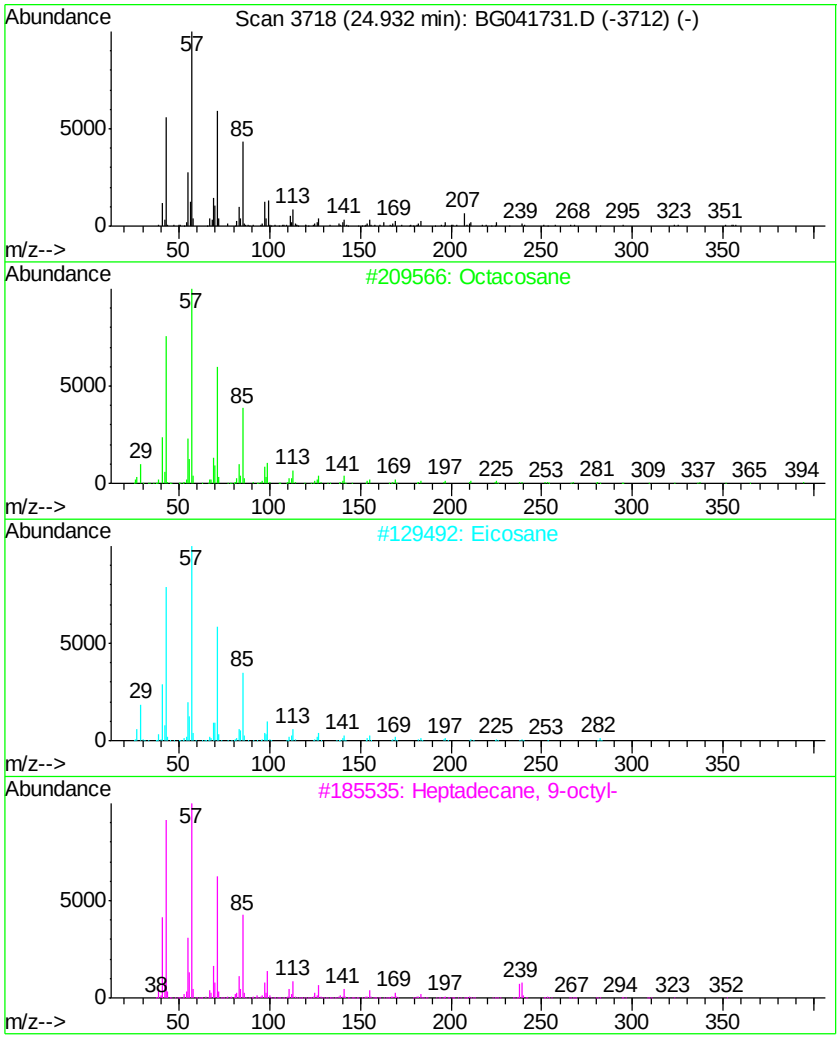
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

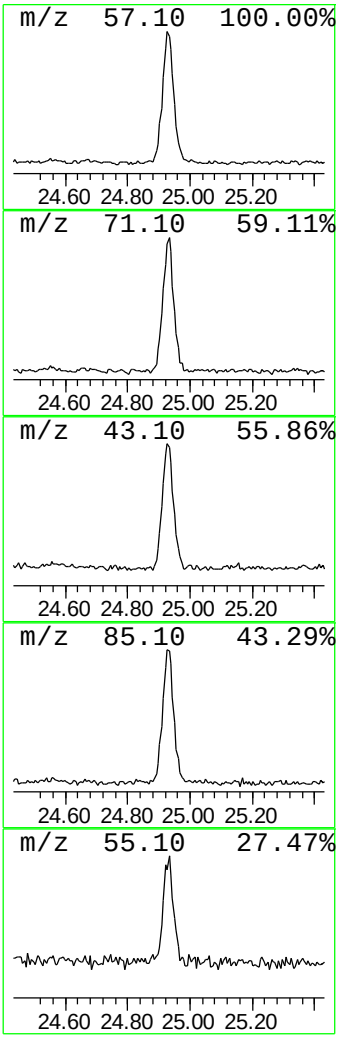
****

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.93	3.85 ng	402633	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Eicosane	282	C20H42	000112-95-8	86
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071919\
Data File : BG041731.D
Acq On : 19 Jul 2019 12:29
Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
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TIC Library : C:\Database\NIST11.L
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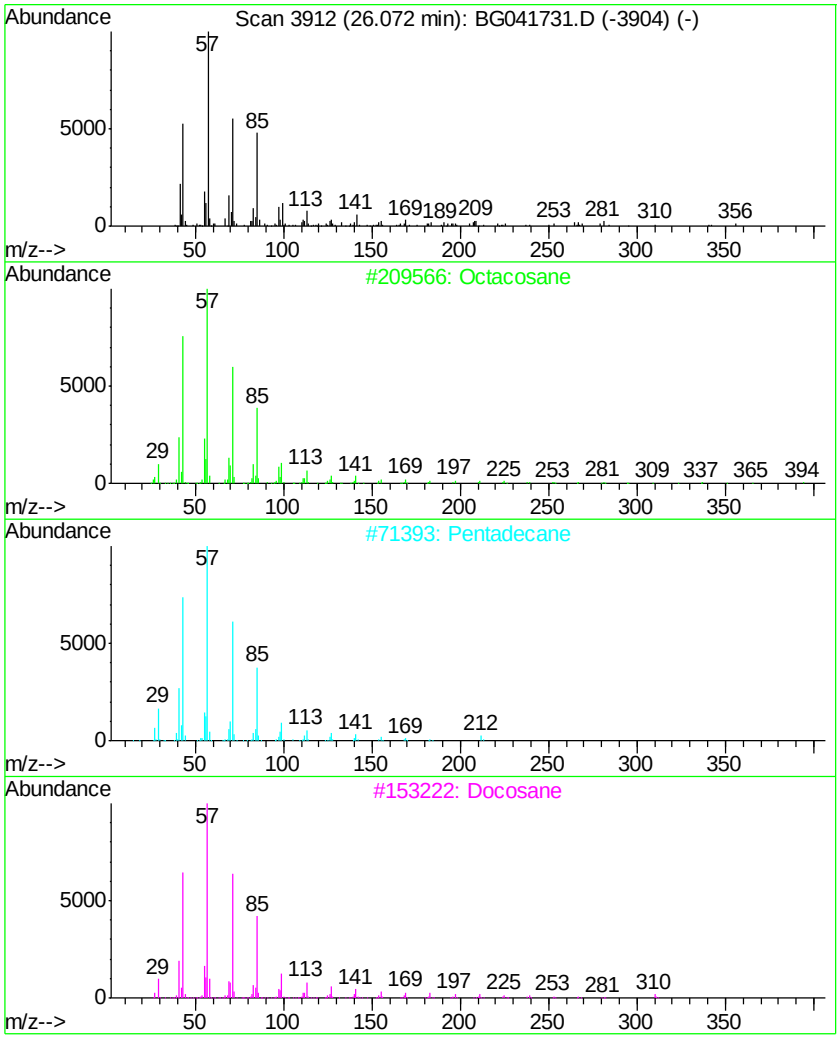
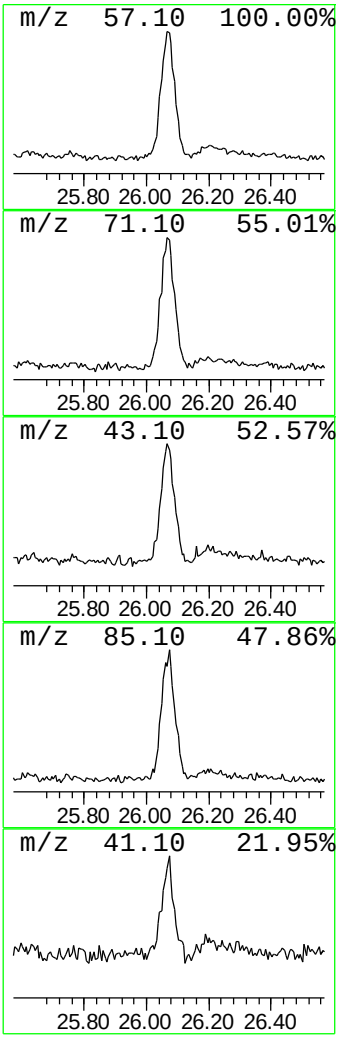
****

Peak Number 11 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.07	3.18 ng	332226	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Docosane	310	C22H46	000629-97-0	83
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
5	Heptadecane	240	C17H36	000629-78-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071919\
Data File : BG041731.D
Acq On : 19 Jul 2019 12:29
Operator : HP/JU
Sample : K3868-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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	16.8	ng	524789	1	8.05	624857	20.0
unknown7.58	7.58	75.7	ng	2366030	1	8.05	624857	20.0
Z-5-Nonadecene	21.31	5.3	ng	537245	5	21.65	2020830	20.0
Eicosane	21.87	2.0	ng	202962	5	21.65	2020830	20.0
unknown21.97	21.97	4.8	ng	488297	5	21.65	2020830	20.0
Lauric anhydride	22.15	5.7	ng	576009	5	21.65	2020830	20.0
Octacosane	23.16	4.4	ng	440326	5	21.65	2020830	20.0
Hexacosane	23.98	4.0	ng	420690	6	24.84	2092030	20.0
Heptadecane, 9-oc...	24.93	3.9	ng	402633	6	24.84	2092030	20.0
Pentadecane	26.07	3.2	ng	332226	6	24.84	2092030	20.0