LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

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-BG042319.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	3.141	3	9	17	rBV	112064	208232	5.60%	0.690%
2	3.217	18	22	35	rVB	236404	324921	8.74%	1.077%
3	5.667	432	439	449	rVB	1076300	1705347	45.87%	5.652%
4	7.277	705	713	729	rBV	1182163	2067089	55.60%	6.851%
5	7.659	770	778	786	rBV	1120164	1902170	51.16%	6.305%
6	8.135	852	859	868	rBV	204441	352482	9.48%	1.168%
7	8.458	906	914	922	rBV	733792	1304419	35.09%	4.323%
8	9.310	1049	1059	1069	rBV	712843	1274164	34.27%	4.223%
9	10.955	1332	1339	1347	rBV	298971	525325	14.13%	1.741%
10	13.388	1745	1753	1763	rVB	1735886	2623520	70.57%	8.695%
11	14.204	1886	1892	1897	rBV	196467	280852	7.55%	0.931%
12	14.763	1979	1987	1998	rBV2	500038	825159	22.19%	2.735%
13	16.249	2232	2240	2248	rBV	1734417	2670856	71.84%	8.852%
14	16.860	2340	2344	2355	rVB7	37076	57858	1.56%	0.192%
15	17.506	2447	2454	2459	rBV	688157	1084796	29.18%	3.595%
16	17.548	2459	2461	2467	rVB	140491	172453	4.64%	0.572%
17	17.636	2470	2476	2481	rBV3	30925	53150	1.43%	0.176%
18	18.229	2573	2577	2584	rBV5	41023	65093	1.75%	0.216%
19	18.364	2593	2600	2607	rBV2	505241	787237	21.17%	2.609%
20	18.423	2607	2610	2616	rVB	63038	104098	2.80%	0.345%
21	18.564	2629	2634	2638	rBV3	66361	114243	3.07%	0.379%
22	18.605	2638	2641	2646	rVB2	40524	60181	1.62%	0.199%
23	18.870	2681	2686	2690	rBV	49553	76170	2.05%	0.252%
24	18.917	2690	2694	2699	rVB3	45188	72421	1.95%	0.240%
25	19.281	2751	2756	2761	rBV5	61792	114347	3.08%	0.379%
26	19.428	2775	2781	2787	rBV3	43662	93655	2.52%	0.310%
27	19.510	2791	2795	2797	rVV5	43414	68601	1.85%	0.227%
28	19.545	2797	2801	2807	rVB	253934	388256	10.44%	1.287%
29	19.622	2807	2814	2823	rBV4	160983	270228	7.27%	0.896%
30	19.698	2823	2827	2831	rVV	44352	66465	1.79%	0.220%
31	19.915	2857	2864	2870	rVB	444615	664720	17.88%	2.203%
32	19.974	2870	2874	2878	rVB4	27578	39585	1.06%	0.131%
33	20.103	2890	2896	2907	rVB	2776514	3717828	100.00%	12.322%
34	20.233	2912	2918	2925	rBV2	50899	113888	3.06%	0.377%

LSC Area Percent Report

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Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

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-BG042319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.368	2934	2941	2942	rBV3	61075	96702	2.60%	0.321%
36	20.556	2969	2973	2977	rBV	71271	86431	2.32%	0.286%
37	20.697	2992	2997	3001	rBV	81926	114991	3.09%	0.381%
38	20.738	3001	3004	3014	rVB	61306	107972	2.90%	0.358%
39	21.161	3073	3076	3084	rVB	40873	73510	1.98%	0.244%
40	21.384	3110	3114	3122	rBV2	208105	377469	10.15%	1.251%
41	21.508	3130	3135	3141	rVB2	27182	63050	1.70%	0.209%
42	21.790	3173	3183	3188	rBV3	768272	1595843	42.92%	5.289%
43	21.837	3188	3191	3197	rVB	174581	270354	7.27%	0.896%
44	22.060	3225	3229	3234	rVB	52993	81380	2.19%	0.270%
45	22.606	3319	3322	3333	rVB8	50213	128095	3.45%	0.425%
46	23.282	3432	3437	3442	rVB6	57718	100548	2.70%	0.333%
47	23.482	3464	3471	3481	rVB	176110	385462	10.37%	1.278%
48	24.058	3562	3569	3575	rBV3	90562	284358	7.65%	0.942%
49	24.821	3693	3699	3710	rVB2	93572	246318	6.63%	0.816%
50	24.974	3717	3725	3733	rVB2	103821	294576	7.92%	0.976%
51	25.139	3740	3753	3763	rBV2	399401	1253017	33.70%	4.153%
52	28.964	4392	4404	4414	rBV5	42931	192401	5.18%	0.638%
53	30.180	4600	4611	4623	rBV4	39175	169247	4.55%	0.561%

Sum of corrected areas: 30171533

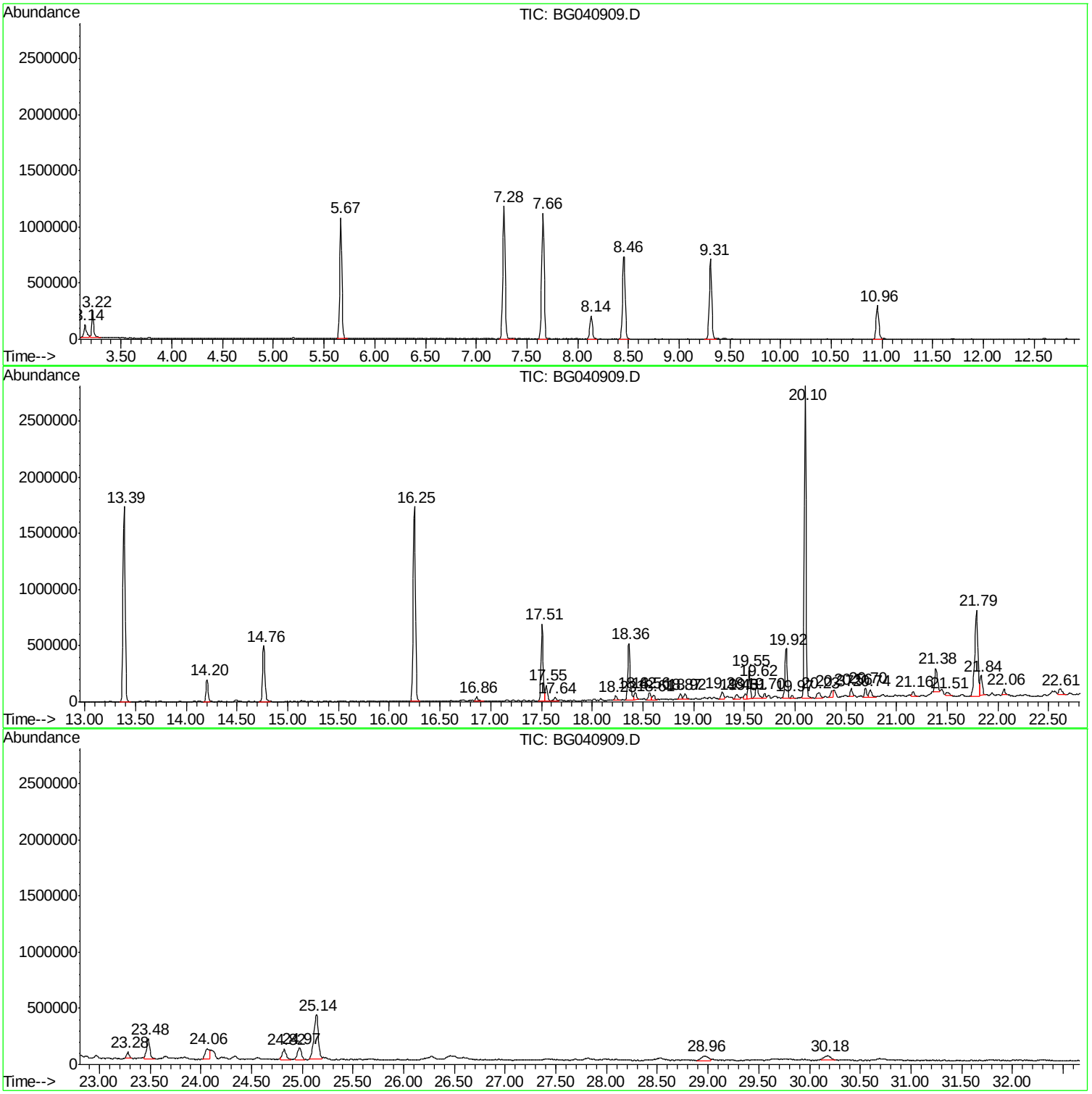
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

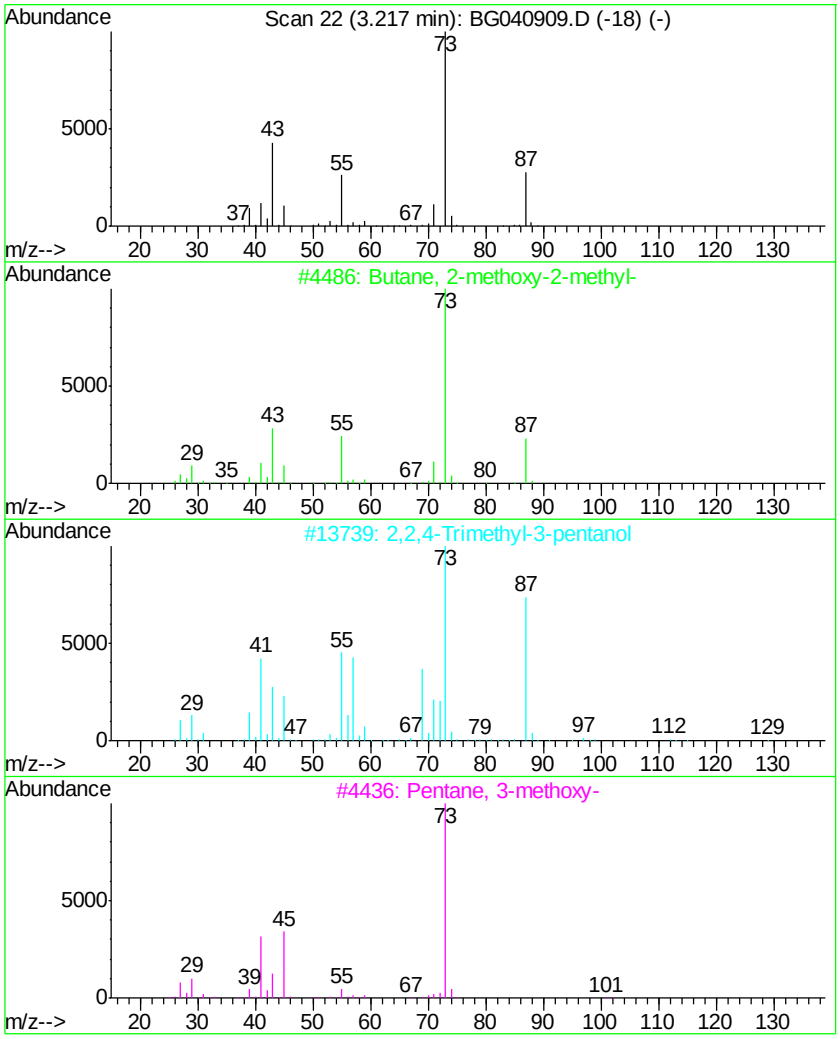
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

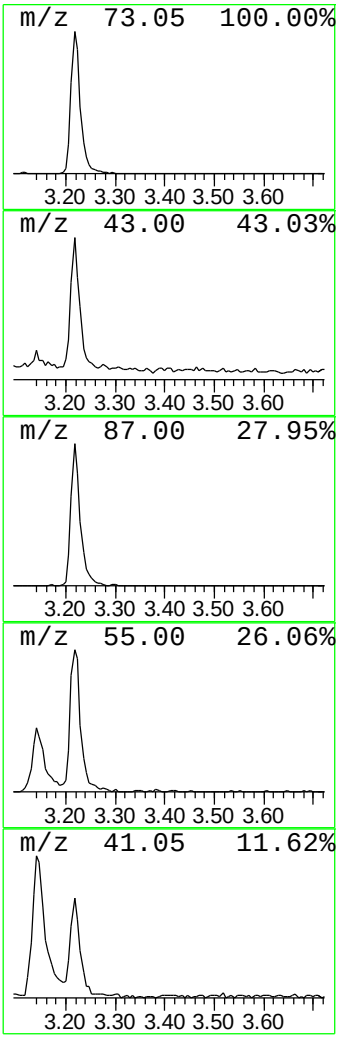
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	18.44 ng	324921	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

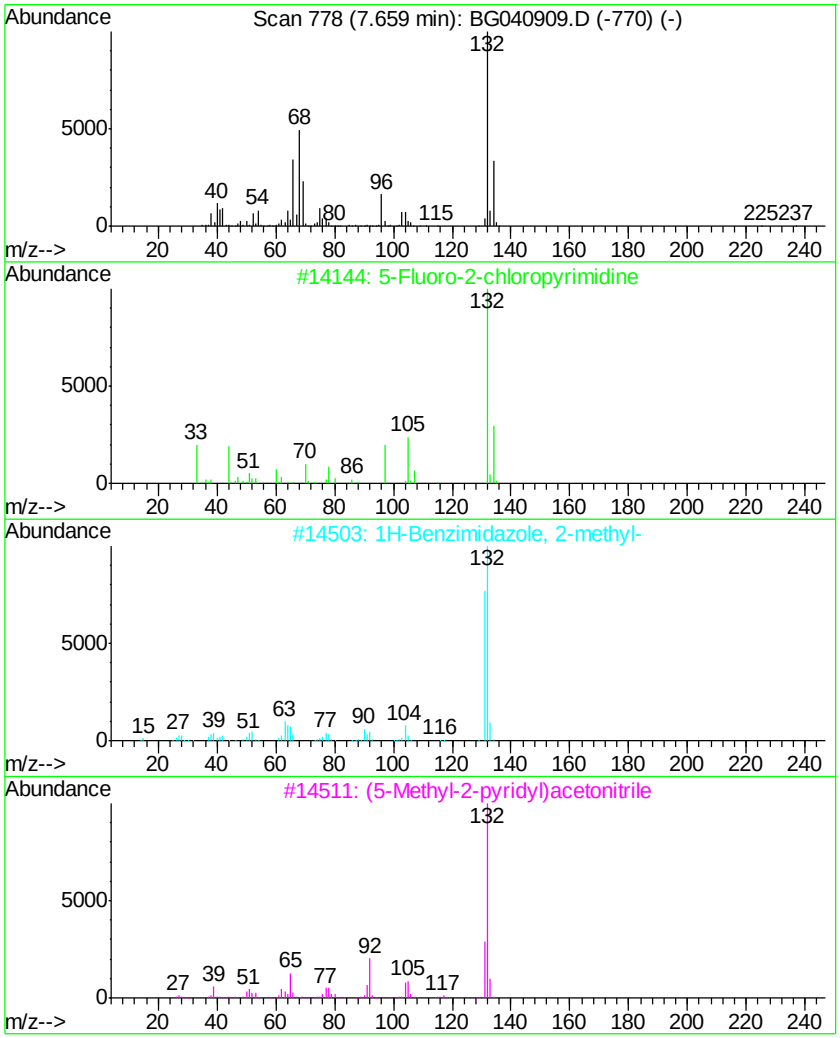
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

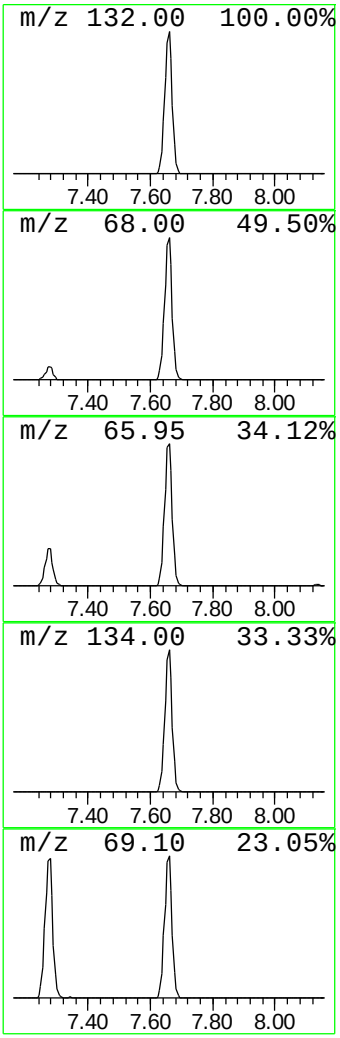
****

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	107.93 ng	1902170	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

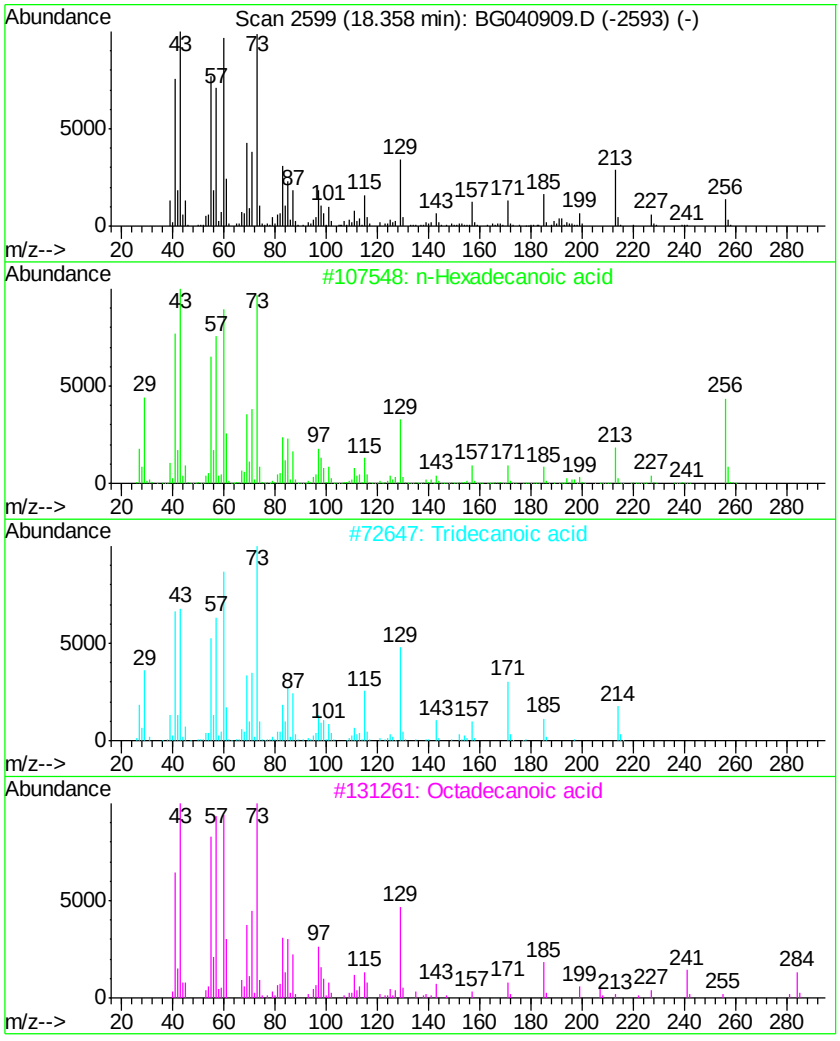
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

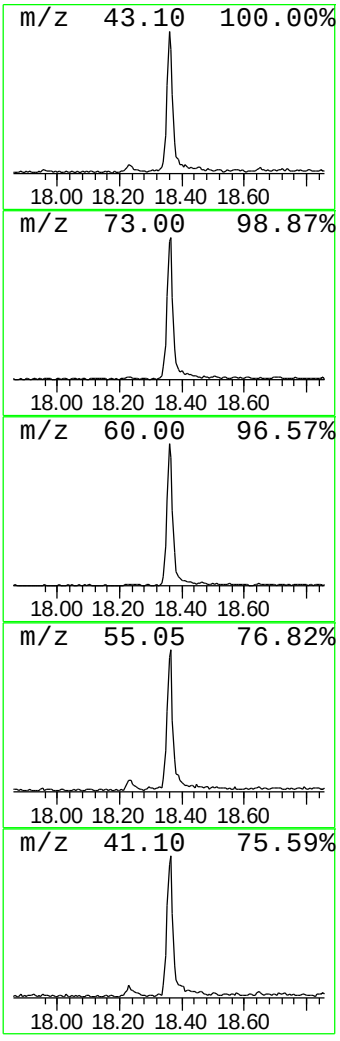
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	14.51 ng	787237	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

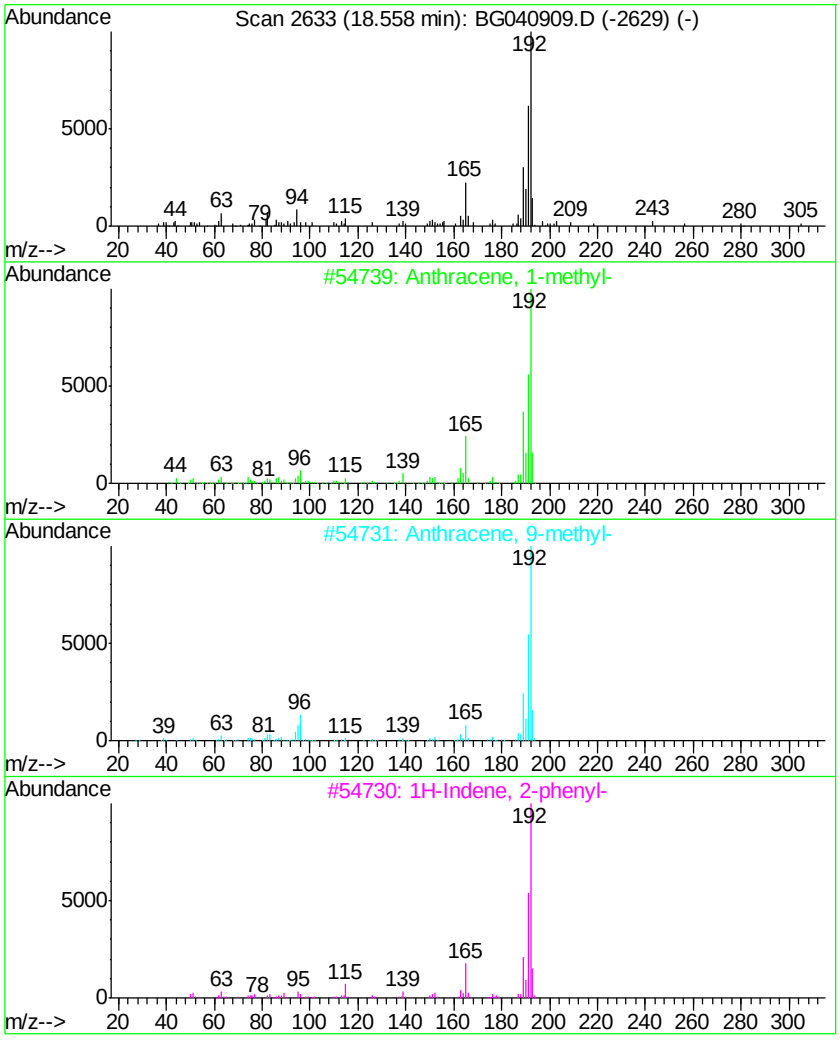
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

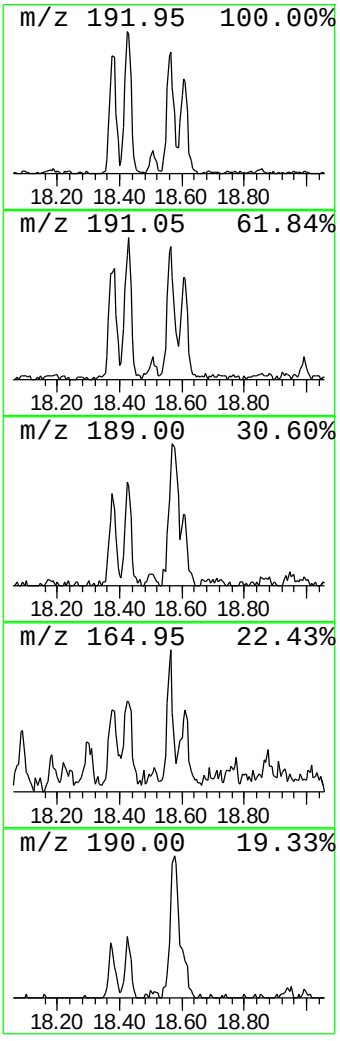
****

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.11 ng	114243	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	76
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	70
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	64





Library Search Compound Report

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Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

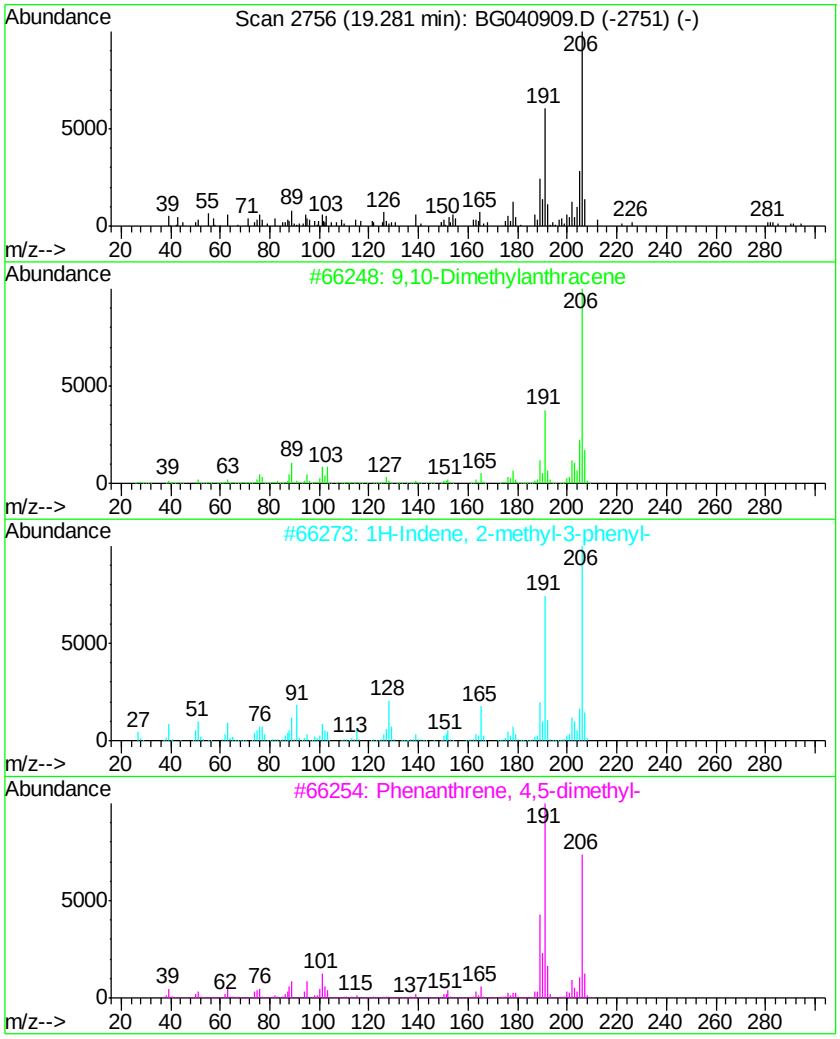
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

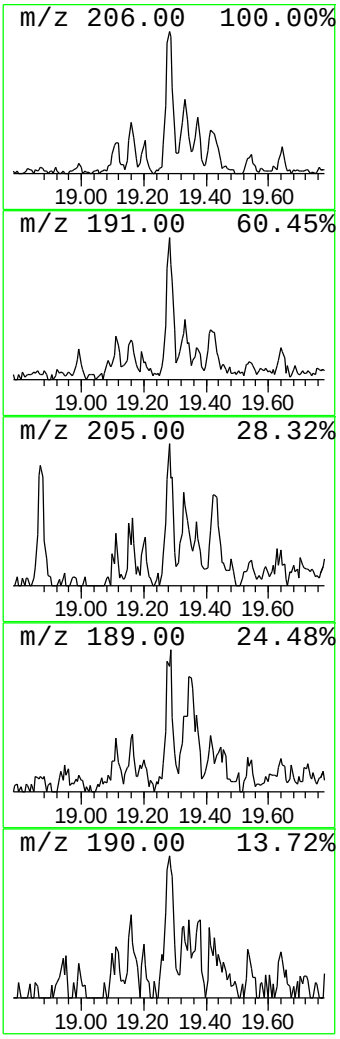
****

Peak Number 7 9,10-Dimethylanthracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	2.11 ng	114347	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
2	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	90
3	Phenanthrene, 4,5-dimethyl-	206	C16H14	003674-69-9	87
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87
5	1,4-Diphenyl-1,3-butadiene	206	C16H14	000886-65-7	76





Library Search Compound Report

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Acq On : 12 May 2019 14:47
Operator : HP/JU
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Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

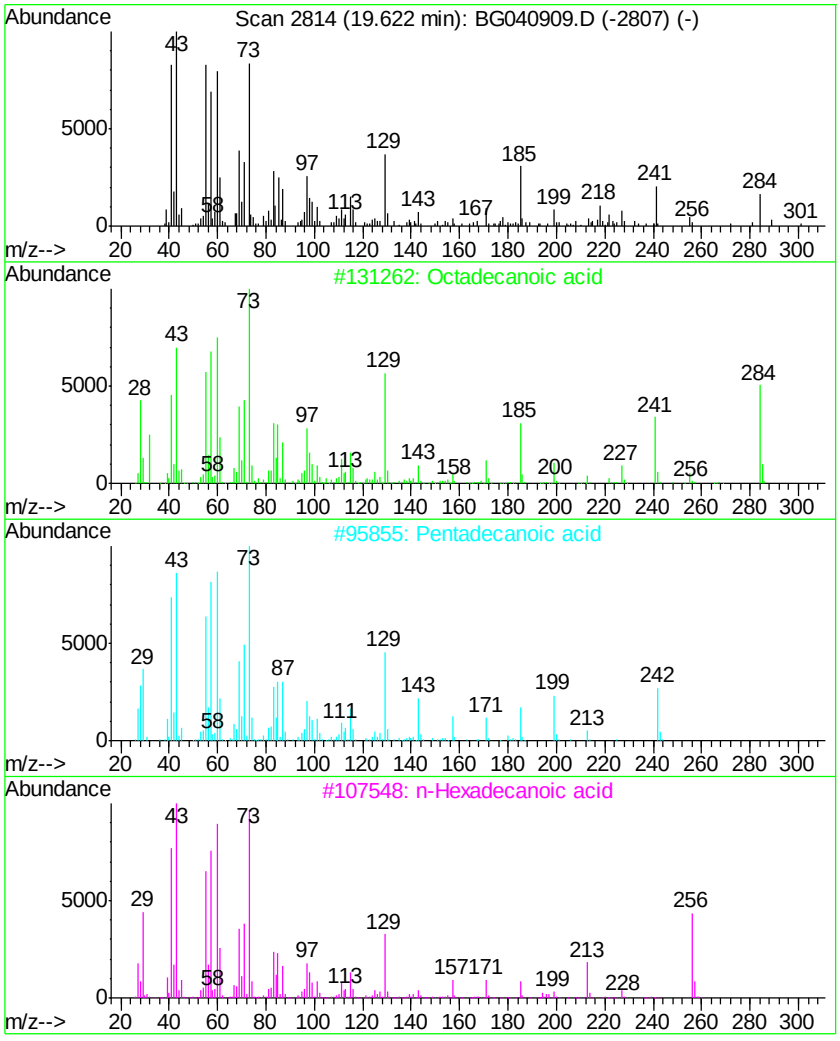
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

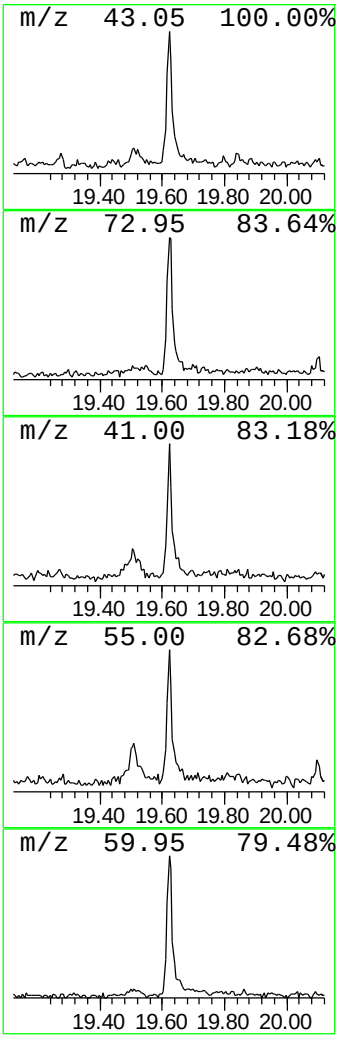
****

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	4.98 ng	270228	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	92
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

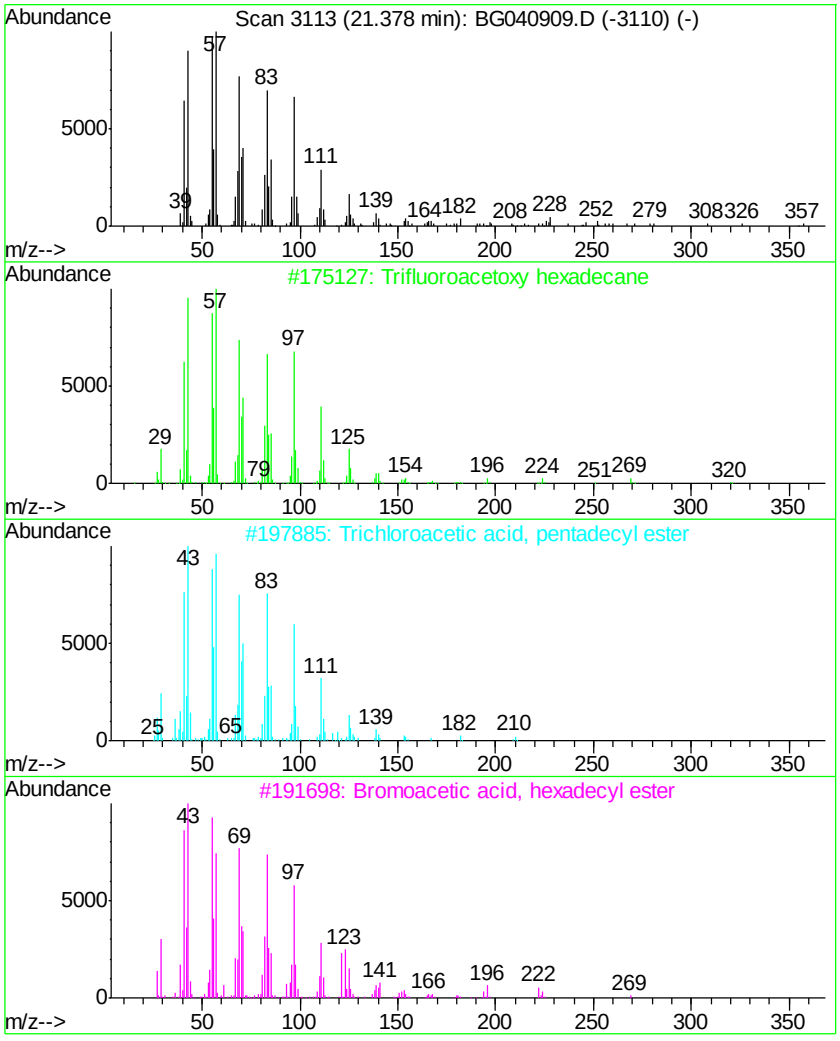
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

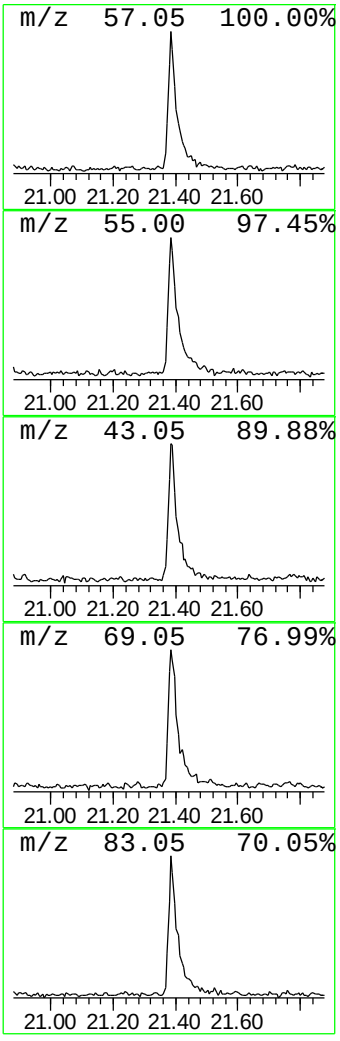
****

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	4.73 ng	377469	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

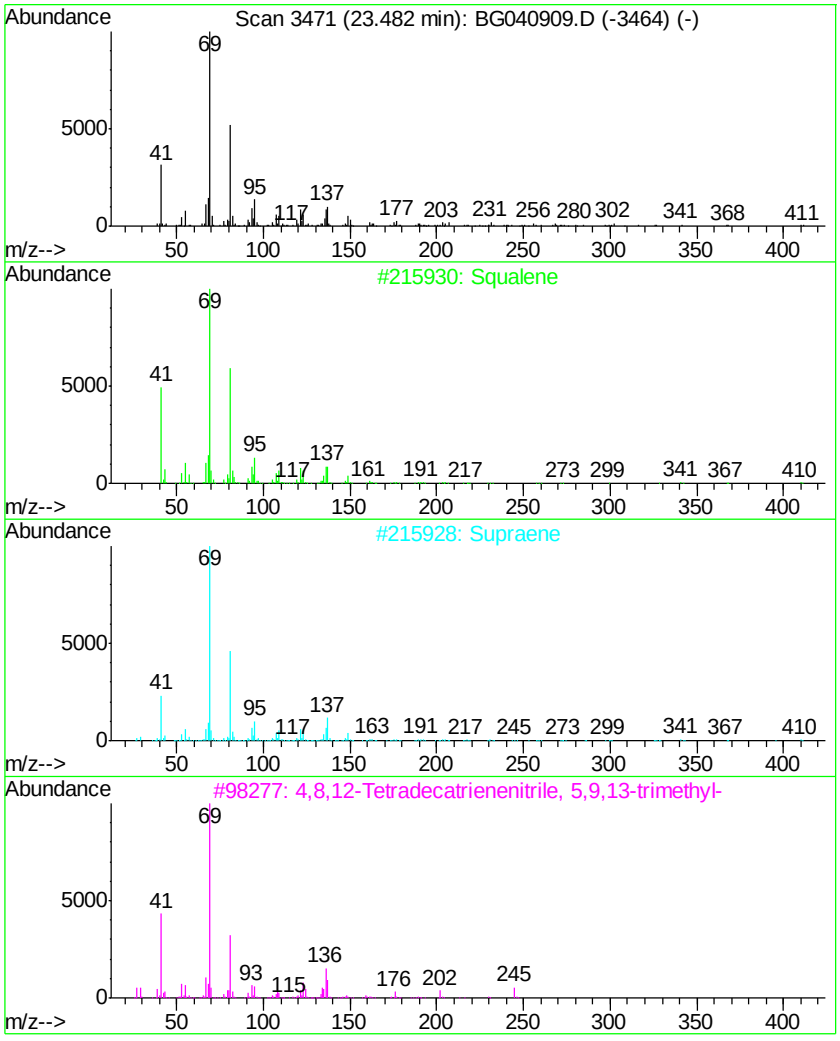
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

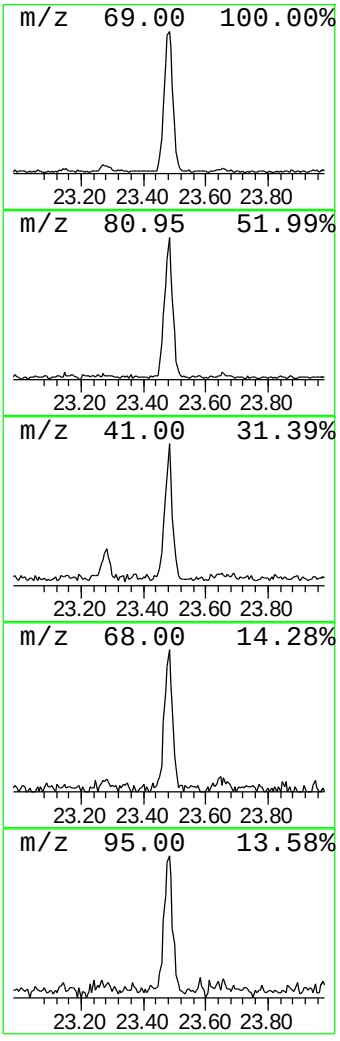
****

Peak Number 10 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.48	6.15 ng	385462	Perylene-d12	25.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	99
2	Supraene	410	C30H50	007683-64-9	99
3	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5	1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040909.D
Acq On : 12 May 2019 14:47
Operator : HP/JU
Sample : K2766-07
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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...	3.22	18.4	ng	324921	1	8.13	352482	20.0
unknown7.66	7.66	107.9	ng	1902170	1	8.13	352482	20.0
n-Hexadecanoic acid	18.36	14.5	ng	787237	4	17.51	1084800	20.0
Anthracene, 1-met...	18.56	2.1	ng	114243	4	17.51	1084800	20.0
9,10-Dimethylanth...	19.28	2.1	ng	114347	4	17.51	1084800	20.0
Octadecanoic acid	19.62	5.0	ng	270228	4	17.51	1084800	20.0
Trifluoroacetoxy ...	21.38	4.7	ng	377469	5	21.79	1595840	20.0
Squalene	23.48	6.2	ng	385462	6	25.14	1253020	20.0