LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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	3.015	26	30	47	rVB	2056210	3042932	94.67%	8.893%
2	4.348	251	257	260	rBV4	27995	46556	1.45%	0.136%
3	5.177	390	398	404	rBV3	39924	70838	2.20%	0.207%
4	5.653	473	479	489	rBV	617119	994574	30.94%	2.907%
5	7.069	715	720	727	rBV6	35569	68580	2.13%	0.200%
6	7.251	744	751	760	rBV2	733576	1275318	39.68%	3.727%
7	7.627	806	815	825	rBV	697245	1225925	38.14%	3.583%
8	8.097	885	895	901	rBV2	469587	844095	26.26%	2.467%
9	8.144	901	903	908	rVB4	44455	55629	1.73%	0.163%
10	8.314	924	932	939	rBV9	38562	95990	2.99%	0.281%
11	8.426	942	951	958	rVB	496920	920591	28.64%	2.691%
12	8.632	979	986	989	rBV5	19314	41058	1.28%	0.120%
13	8.755	1003	1007	1012	rVB5	23584	36446	1.13%	0.107%
14	9.266	1087	1094	1102	rVB	471000	851155	26.48%	2.488%
15	10.012	1213	1221	1226	rBV2	99892	162357	5.05%	0.475%
16	10.147	1238	1244	1249	rBV8	23200	57851	1.80%	0.169%
17	10.371	1279	1282	1288	rBV8	14959	33014	1.03%	0.096%
18	10.923	1369	1376	1383	rVB	685040	1276642	39.72%	3.731%
19	11.375	1446	1453	1458	rBV4	46364	74919	2.33%	0.219%
20	13.021	1728	1733	1739	rVB8	21682	49371	1.54%	0.144%
21	13.355	1783	1790	1797	rBV	1374673	2227620	69.30%	6.510%
22	14.178	1924	1930	1939	rBV	298231	456555	14.20%	1.334%
23	14.736	2017	2025	2033	rVB2	1271555	2108428	65.59%	6.162%
24	15.130	2088	2092	2096	rBV5	80258	102089	3.18%	0.298%
25	15.212	2101	2106	2113	rVV2	178533	253482	7.89%	0.741%
26	15.283	2113	2118	2125	rVB5	20666	39738	1.24%	0.116%
27	15.500	2150	2155	2157	rVV5	23968	36929	1.15%	0.108%
28	15.547	2159	2163	2168	rVB3	52032	76807	2.39%	0.224%
29	16.223	2271	2278	2285	rBV	1147221	1805413	56.17%	5.277%
30	16.411	2304	2310	2321	rBV7	72874	166125	5.17%	0.486%
31	16.546	2330	2333	2336	rBV	56065	72765	2.26%	0.213%
32	16.599	2338	2342	2348	rVV5	65830	114928	3.58%	0.336%
33	16.663	2348	2353	2358	rVV4	50952	90977	2.83%	0.266%
34	16.804	2373	2377	2382	rVB6	30797	42438	1.32%	0.124%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.869	2382	2388	2393	rVB9	41278	86271	2.68%	0.252%
36	16.928	2393	2398	2403	rBV2	58955	104581	3.25%	0.306%
37	17.204	2440	2445	2448	rBV4	62537	95377	2.97%	0.279%
38	17.480	2484	2492	2498	rBV2	1526974	2450076	76.22%	7.161%
39	17.533	2499	2501	2505	rVB4	30263	33134	1.03%	0.097%
40	17.850	2549	2555	2559	rVB8	19932	41821	1.30%	0.122%
41	18.115	2596	2600	2606	rVB9	36144	62888	1.96%	0.184%
42	18.338	2633	2638	2647	rBV2	428175	659177	20.51%	1.927%
43	18.408	2648	2650	2654	rVB4	26325	36607	1.14%	0.107%
44	19.460	2826	2829	2832	rBV4	45700	68373	2.13%	0.200%
45	19.501	2832	2836	2842	rVB7	117262	171270	5.33%	0.501%
46	19.595	2849	2852	2855	rBV5	75699	97635	3.04%	0.285%
47	19.760	2876	2880	2883	rBV	49291	61211	1.90%	0.179%
48	20.065	2927	2932	2938	rVB	2491117	3214329	100.00%	9.394%
49	20.735	3040	3046	3061	rVB2	294622	689191	21.44%	2.014%
50	21.740	3211	3217	3224	rVB2	1585538	2667838	83.00%	7.797%
51	21.834	3229	3233	3238	rBV5	116058	191851	5.97%	0.561%
52	23.203	3459	3466	3479	rBV2	1127782	2360928	73.45%	6.900%
53	25.024	3766	3776	3787	rBV2	768662	2305346	71.72%	6.738%

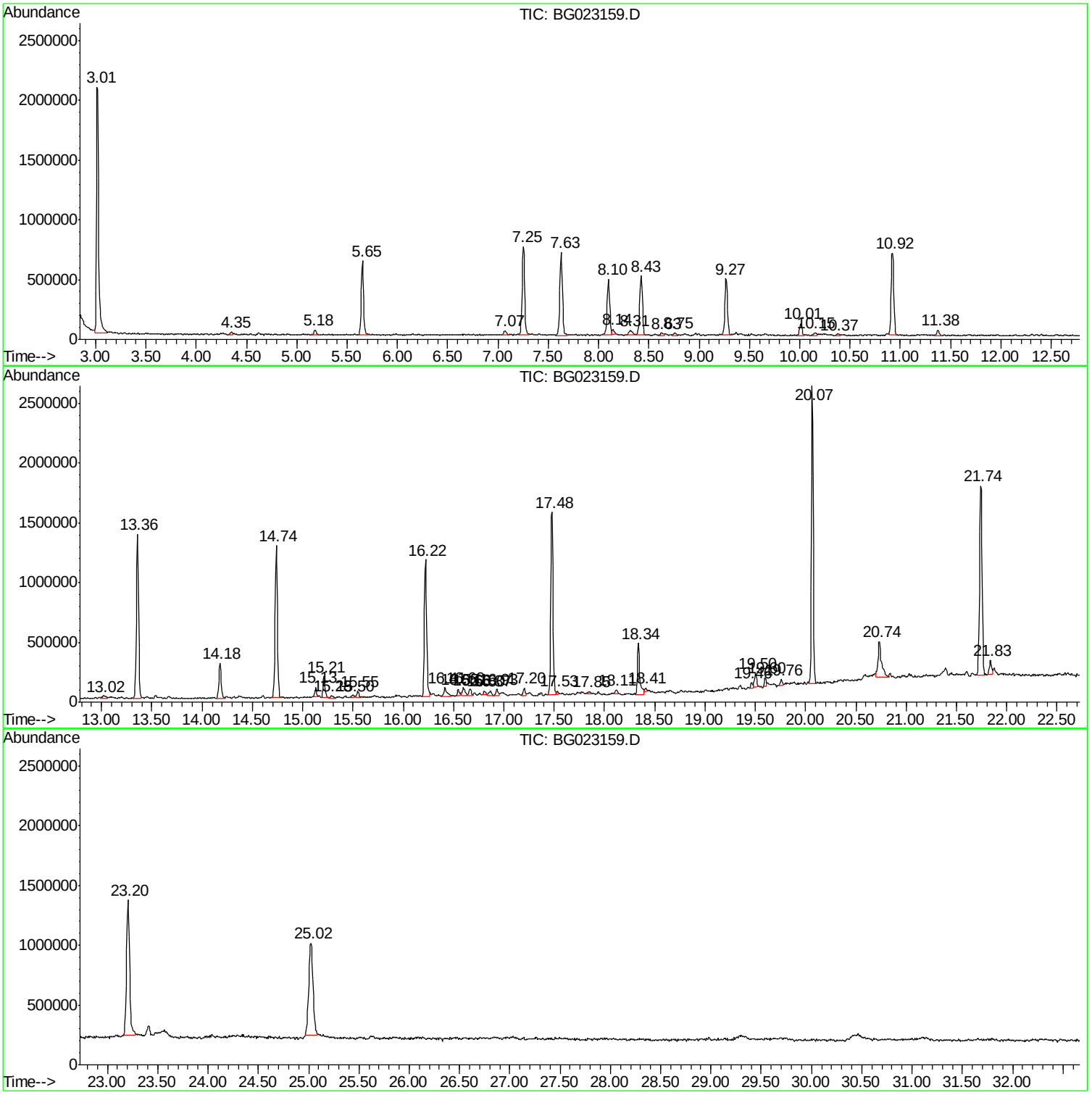
Sum of corrected areas: 34216039

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

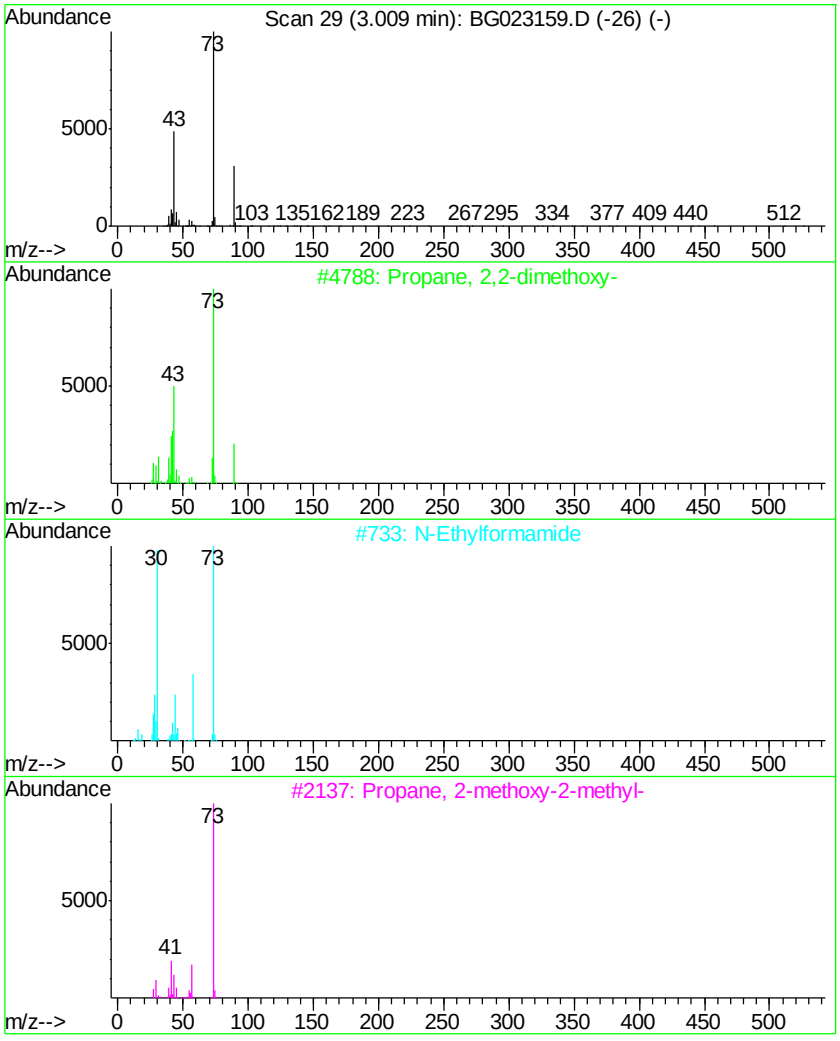
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

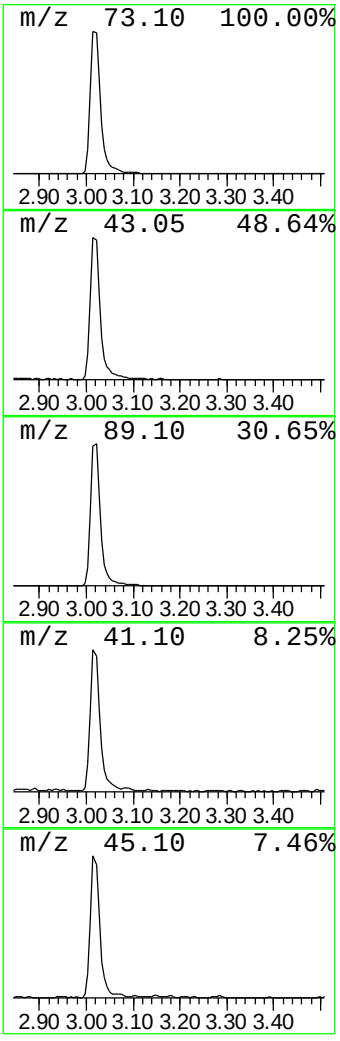
****

Peak Number 1 unknown3.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	72.10 ng	3042930	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

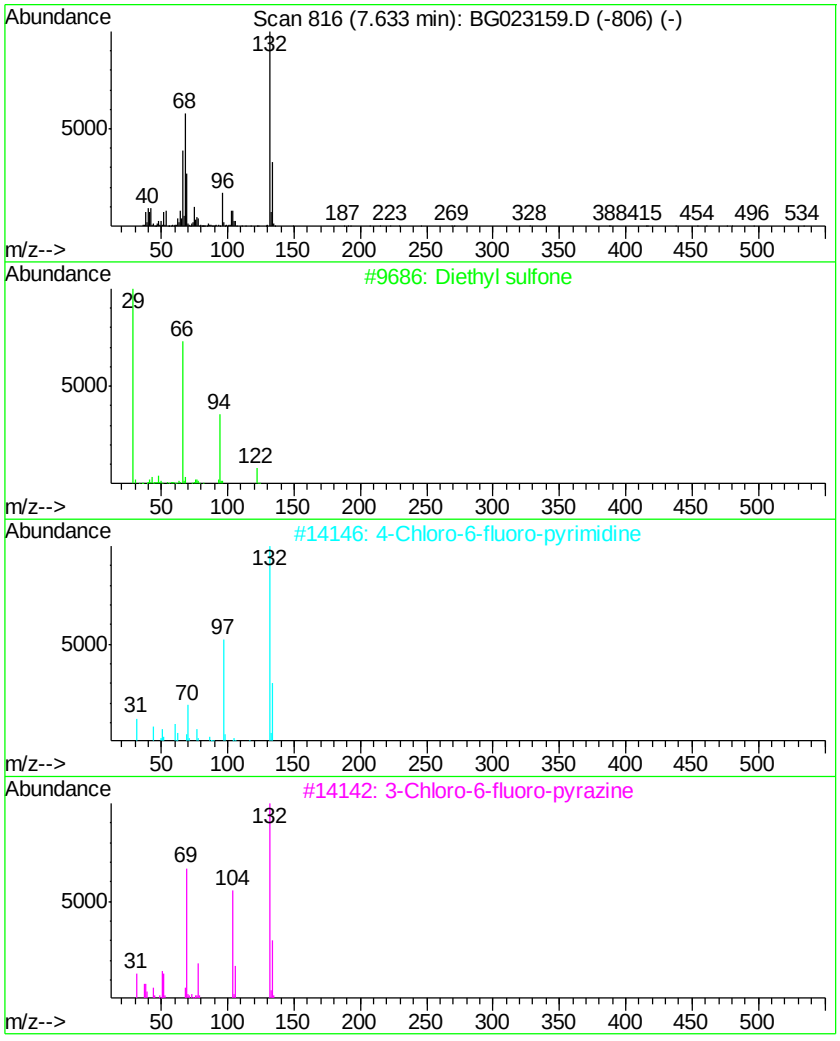
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

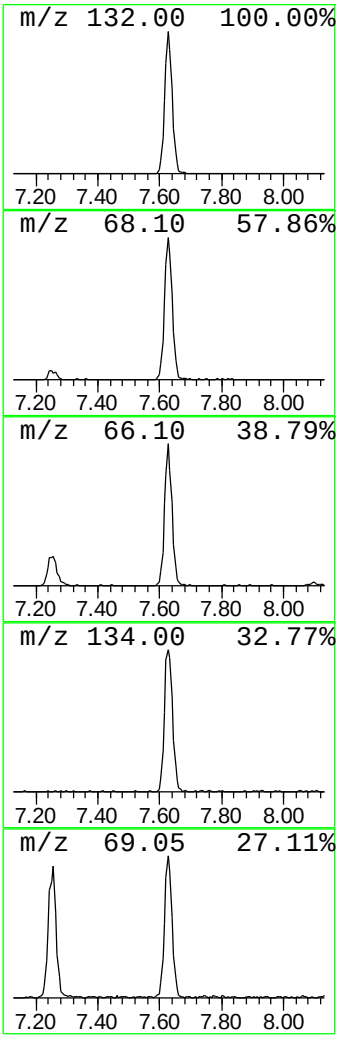
****

Peak Number 2 unknown7.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	29.05 ng	1225930	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfone	122	C4H10O2S	000597-35-3	17
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

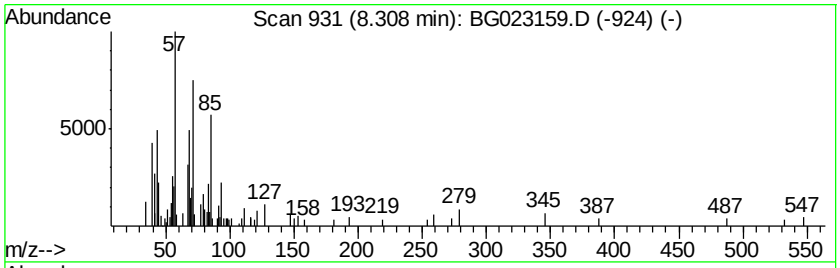
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

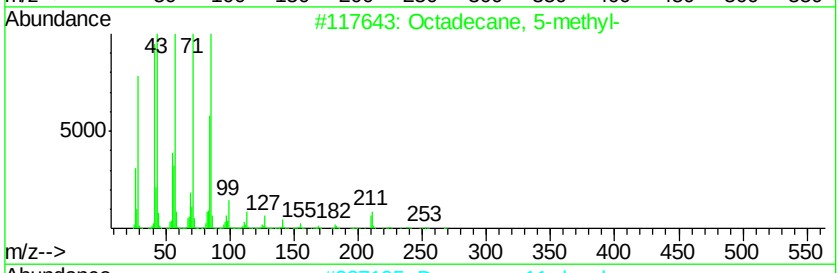
****

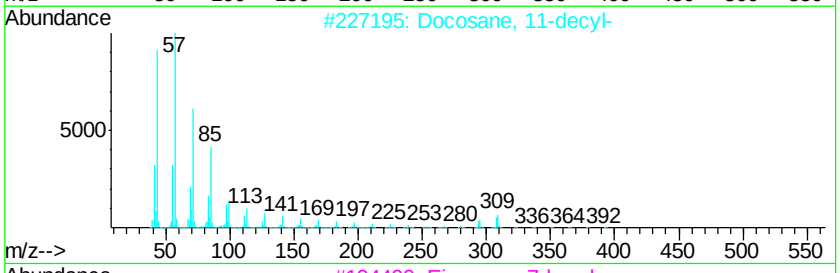
Peak Number 3 unknown8.31 Concentration Rank 9

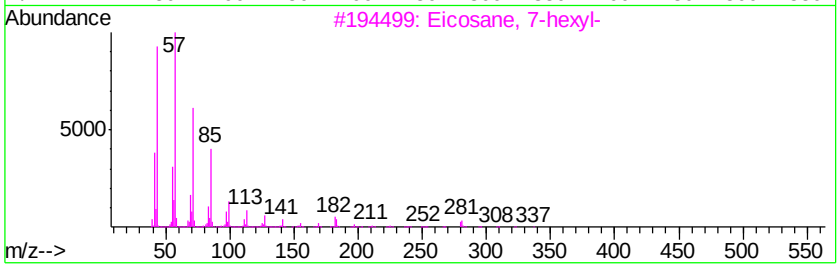
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.31	2.27 ng	95990	1,4-Dichlorobenzene-d4	8.10

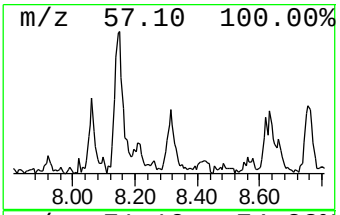
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 5-methyl-	268	C19H40	025117-35-5	38
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	35
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	35
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	35
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	35

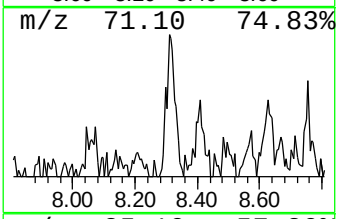


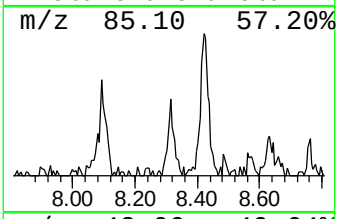


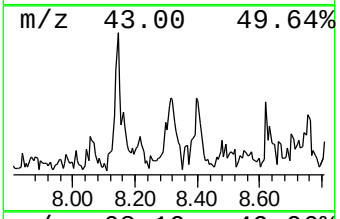


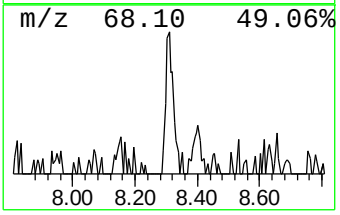












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Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

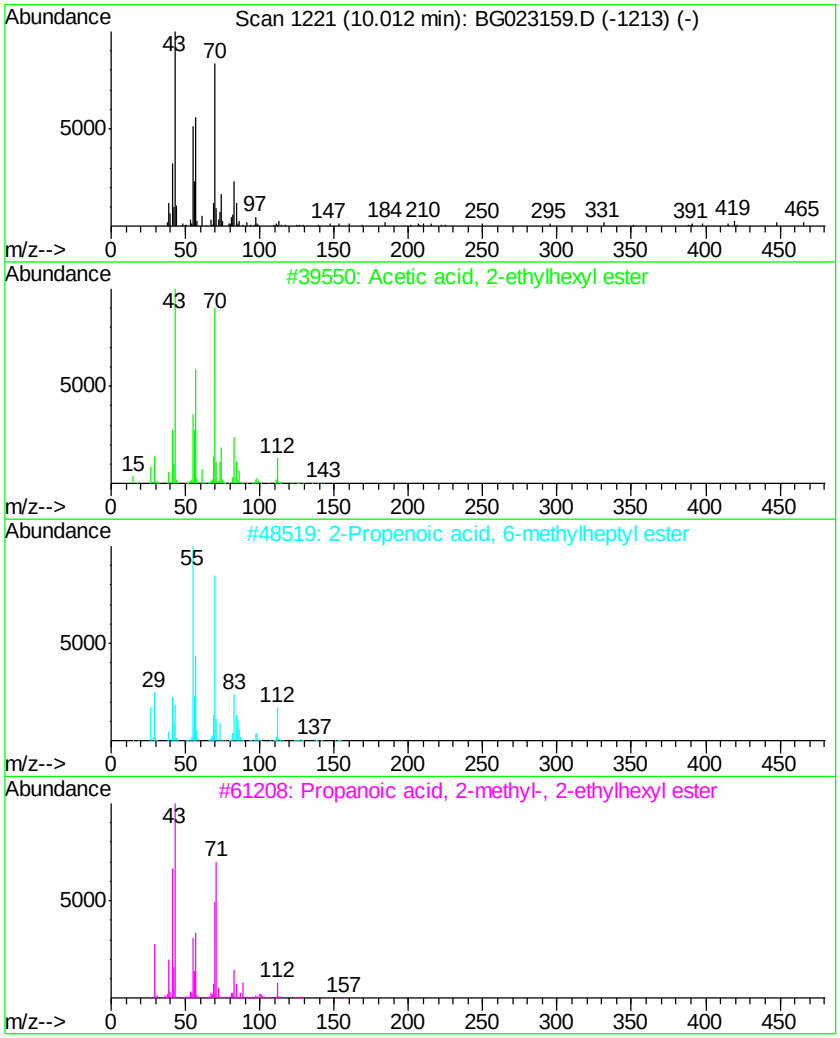
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

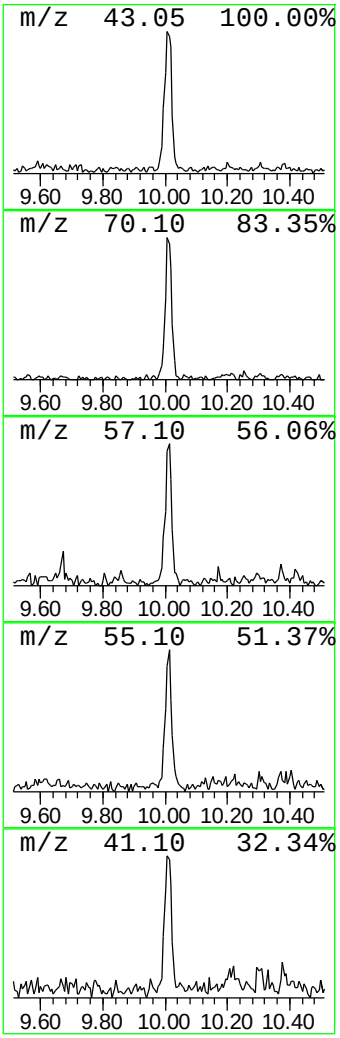
****

Peak Number 5 Acetic acid, 2-ethylhexyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.01	2.54 ng	162357	Naphthalene-d8	10.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	86
2	2-Propenoic acid, 6-methylheptyl...	184	C11H20O2	054774-91-3	78
3	Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	64
4	4-(Prop-2-enoyloxy)octane	184	C11H20O2	042928-87-0	64
5	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	64





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

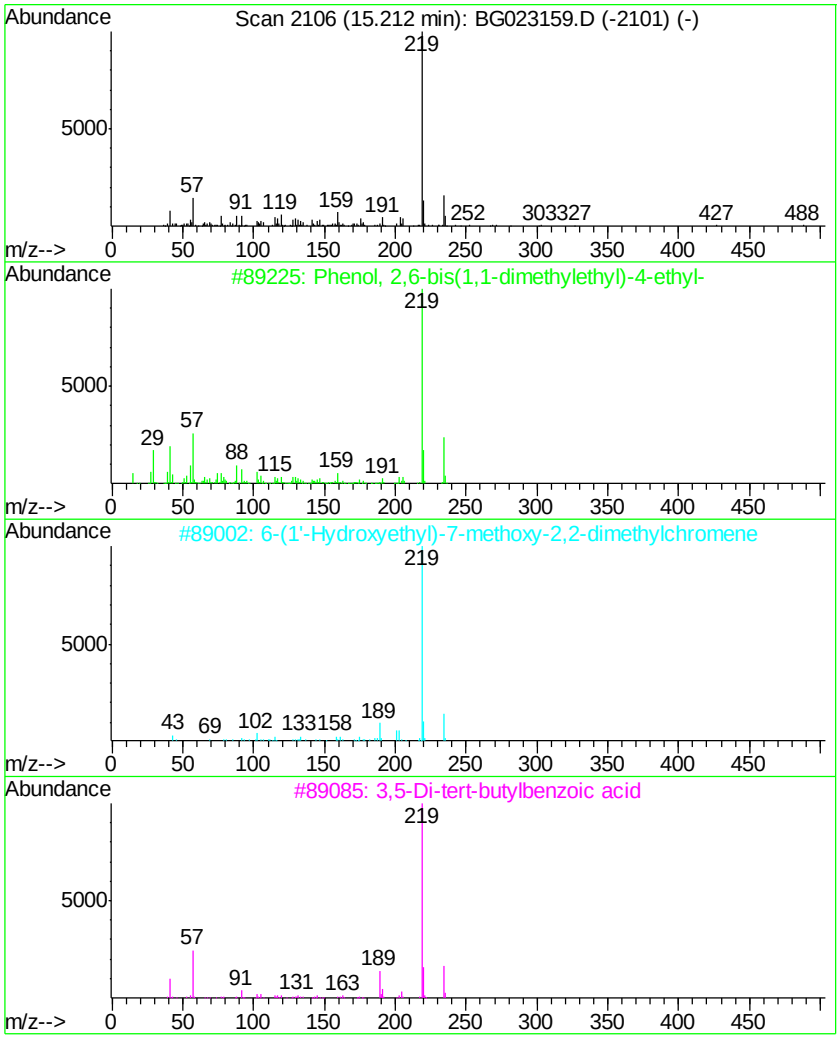
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

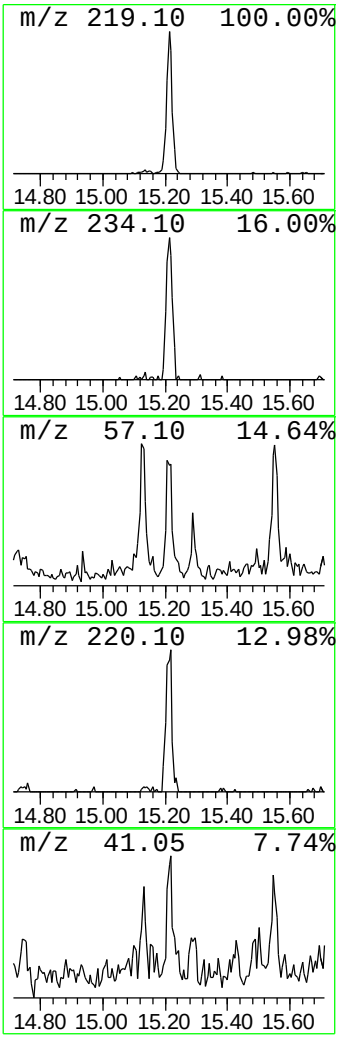
****

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.40 ng	253482	Acenaphthene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91
2	6-(1'-Hydroxyethyl)-7-methoxy-2,...	234	C14H18O3	1000360-28-8	72
3	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	72
4	Quinoline, 2-(3-tolyl)-	219	C16H13N	024641-30-3	58
5	Indole-3-carboxylic acid, 5-hydr...	219	C12H13NO3	073975-59-4	53





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Data File : BG023159.D
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Sample : H4061-01
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Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

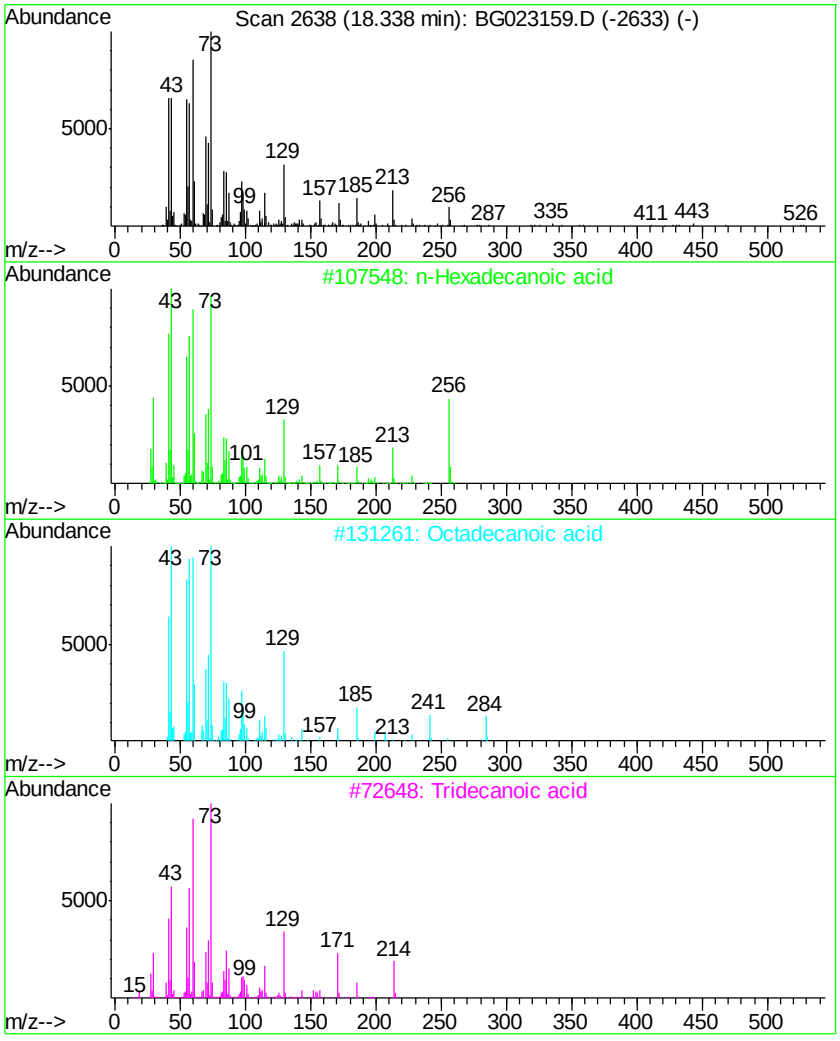
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

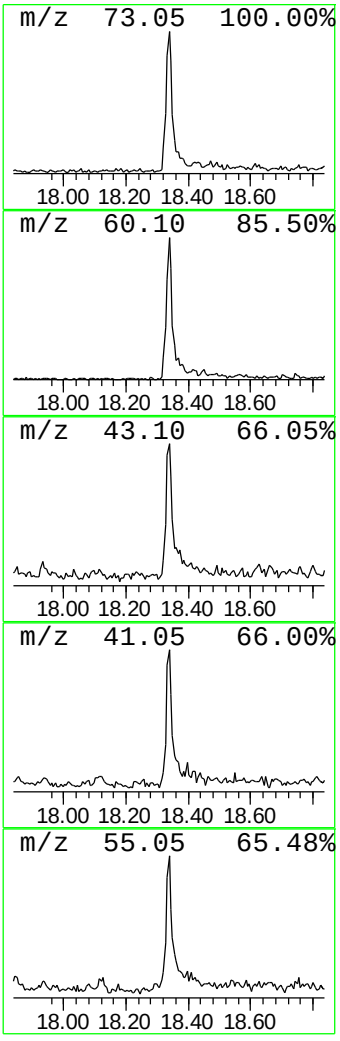
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	5.38 ng	659177	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

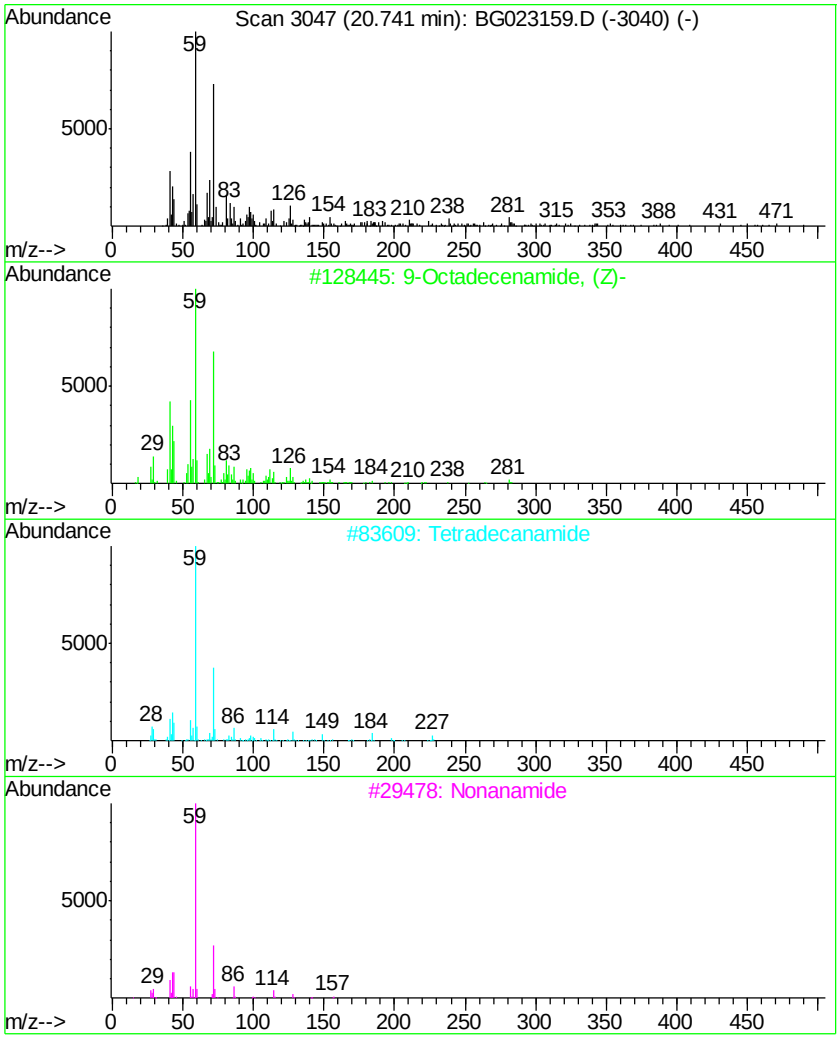
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

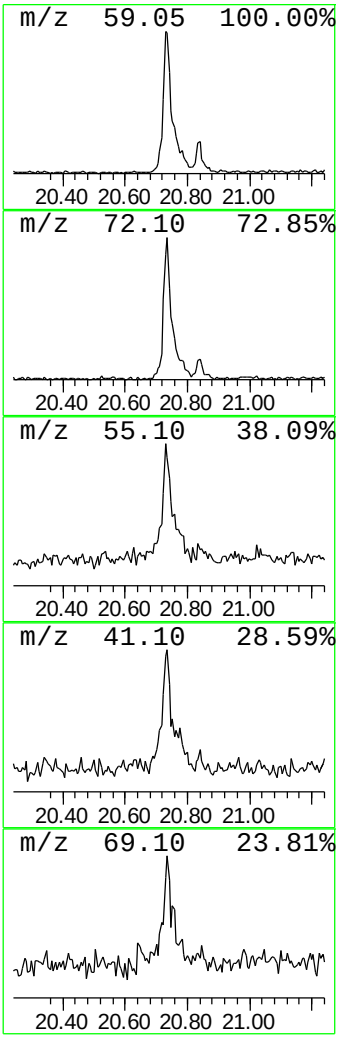
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.74	5.17 ng	689191	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Nonanamide	157	C9H19NO	001120-07-6	47
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	Hexanamide	115	C6H13NO	000628-02-4	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

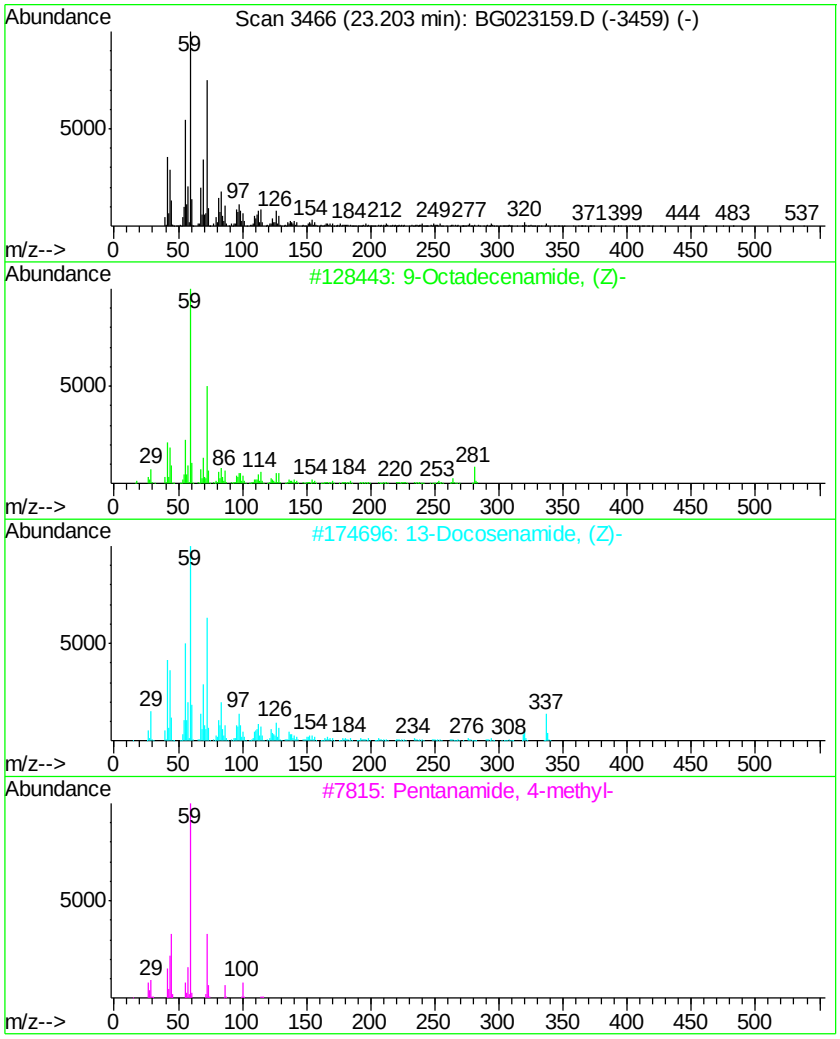
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

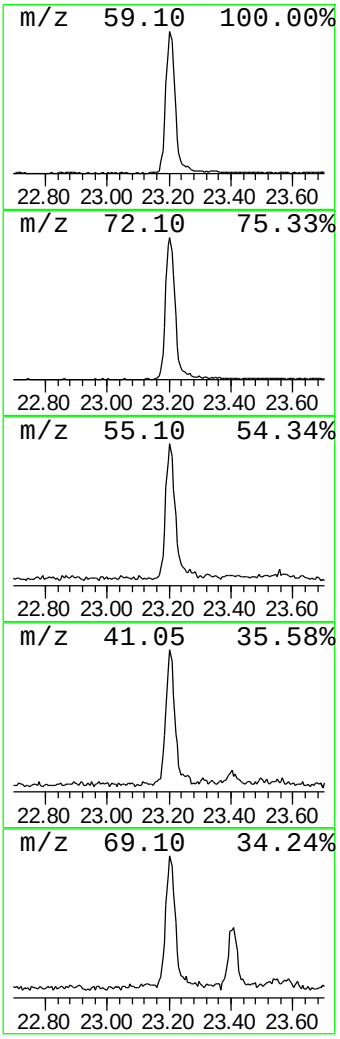
****

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	17.70 ng	2360930	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
4	Dodecanamide	199	C12H25NO	001120-16-7	38
5	2-Propanone, 1-cyclopentyl-	126	C8H14O	001122-98-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071816\
Data File : BG023159.D
Acq On : 18 Jul 2016 13:55
Operator : UM/SJ
Sample : H4061-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1607084522-23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
unknown3.01	3.01	72.1	ng	3042930	1	8.10	844095	20.0
unknown7.63	7.63	29.1	ng	1225930	1	8.10	844095	20.0
unknown8.31	8.31	2.3	ng	95990	1	8.10	844095	20.0
Acetic acid, 2-et...	10.01	2.5	ng	162357	2	10.92	1276640	20.0
Phenol, 2,6-bis(1...	15.21	2.4	ng	253482	3	14.74	2108430	20.0
n-Hexadecanoic acid	18.34	5.4	ng	659177	4	17.48	2450080	20.0
9-Octadecenamide,...	20.74	5.2	ng	689191	5	21.74	2667840	20.0
13-Docosenamide, ...	23.20	17.7	ng	2360930	5	21.74	2667840	20.0