LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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-BG042315.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	2.723	3	6	11	rVB	125678	150019	5.67%	0.715%
2	4.680	331	339	349	rBV	195492	270058	10.20%	1.287%
3	5.167	416	422	437	rBV	960401	1348137	50.94%	6.424%
4	6.777	689	696	708	rBV	962787	1464545	55.34%	6.979%
5	7.112	746	753	764	rBV	1037270	1559194	58.92%	7.430%
6	7.570	825	831	839	rVB	252652	379912	14.36%	1.810%
7	7.888	877	885	897	rBV	766222	1172113	44.29%	5.585%
8	8.734	1019	1029	1040	rBV	538808	884727	33.43%	4.216%
9	10.355	1295	1305	1318	rBV	339755	574588	21.71%	2.738%
10	12.841	1721	1728	1739	rBV	1451293	2001733	75.64%	9.539%
11	13.693	1867	1873	1881	rBV	46295	71909	2.72%	0.343%
12	14.227	1957	1964	1971	rBV2	522623	811585	30.67%	3.867%
13	15.720	2212	2218	2231	rBV	1007534	1380303	52.16%	6.578%
14	15.943	2251	2256	2264	rBV2	18869	34982	1.32%	0.167%
15	16.971	2425	2431	2435	rBV	694963	943583	35.65%	4.496%
16	17.012	2435	2438	2444	rVB	93712	121548	4.59%	0.579%
17	17.100	2449	2453	2460	rVB2	26579	39109	1.48%	0.186%
18	17.876	2581	2585	2598	rVB3	104753	191121	7.22%	0.911%
19	18.040	2606	2613	2617	rBV3	25862	47837	1.81%	0.228%
20	19.033	2776	2782	2791	rBV	281500	379424	14.34%	1.808%
21	19.163	2800	2804	2813	rBV4	35668	57316	2.17%	0.273%
22	19.304	2824	2828	2833	rVB	187074	207534	7.84%	0.989%
23	19.398	2834	2844	2853	rVV	229304	423031	15.98%	2.016%
24	19.603	2872	2879	2894	rBV	2052901	2646508	100.00%	12.611%
25	19.721	2894	2899	2906	rVB6	21447	48342	1.83%	0.230%
26	19.891	2925	2928	2937	rVB2	37641	69760	2.64%	0.332%
27	20.050	2949	2955	2960	rVB3	26706	44806	1.69%	0.214%
28	20.244	2983	2988	2991	rBV2	18435	29812	1.13%	0.142%
29	20.349	3002	3006	3011	rVB	150978	170450	6.44%	0.812%
30	20.414	3011	3017	3020	rBV	35895	46805	1.77%	0.223%
31	20.449	3020	3023	3026	rVV4	28420	29162	1.10%	0.139%
32	20.643	3052	3056	3062	rVB	25073	33108	1.25%	0.158%
33	20.872	3092	3095	3101	rVB4	151242	204841	7.74%	0.976%
34	21.154	3137	3143	3148	rBV2	805058	1232742	46.58%	5.874%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

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-BG042315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.196	3148	3150	3159	rVB	122339	145089	5.48%	0.691%
36	21.307	3166	3169	3175	rBV	72026	84546	3.19%	0.403%
37	21.730	3238	3241	3252	rVB2	52839	87044	3.29%	0.415%
38	22.177	3314	3317	3321	rBV2	48969	65322	2.47%	0.311%
39	22.306	3336	3339	3344	rVB2	37464	49617	1.87%	0.236%
40	22.694	3398	3405	3411	rBV2	97661	281532	10.64%	1.342%
41	23.164	3481	3485	3490	rVB2	58162	102919	3.89%	0.490%
42	23.252	3497	3500	3507	rVB	81619	139932	5.29%	0.667%
43	23.358	3511	3518	3523	rBV	524800	958520	36.22%	4.568%

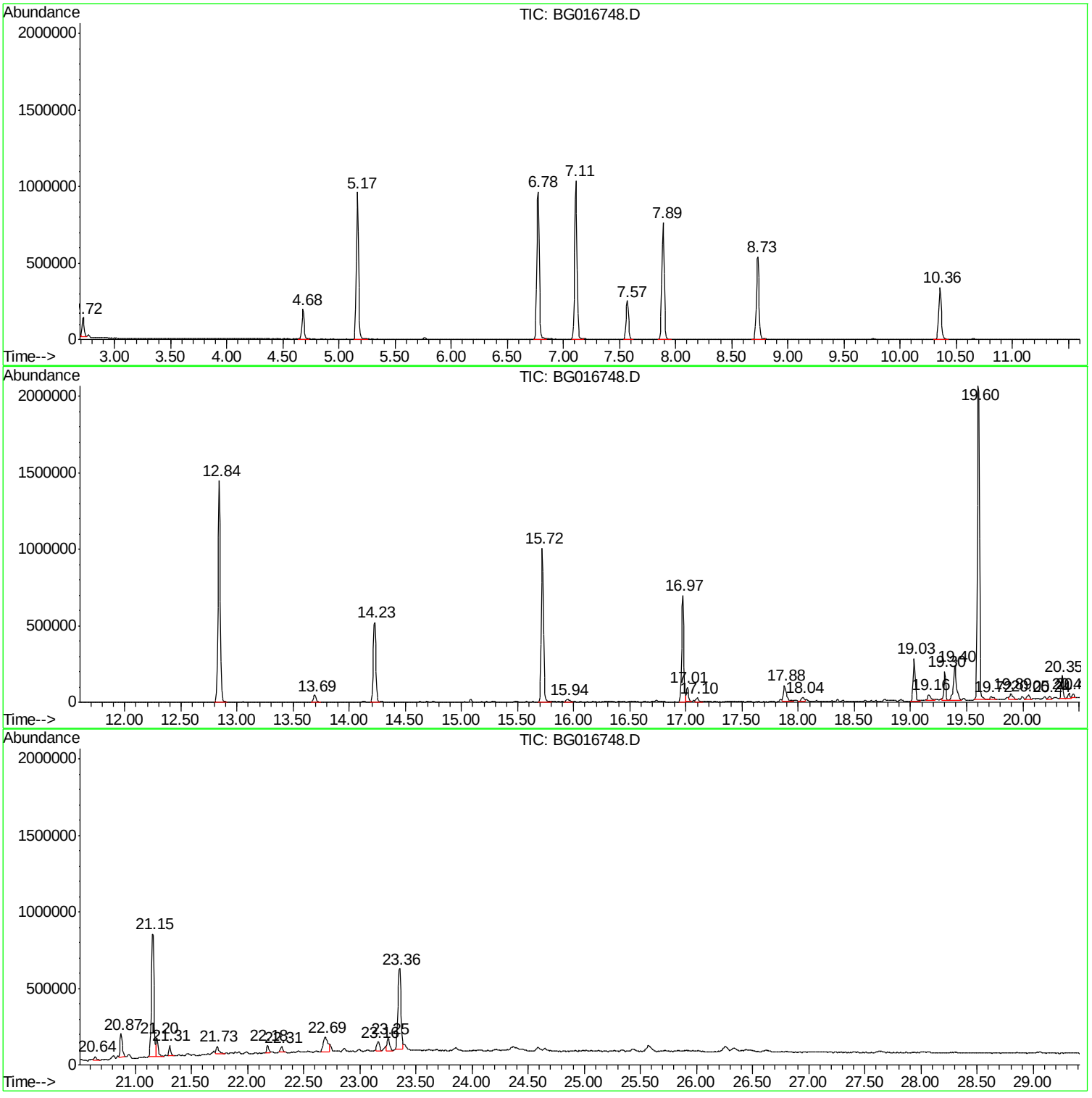
Sum of corrected areas: 20985165

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

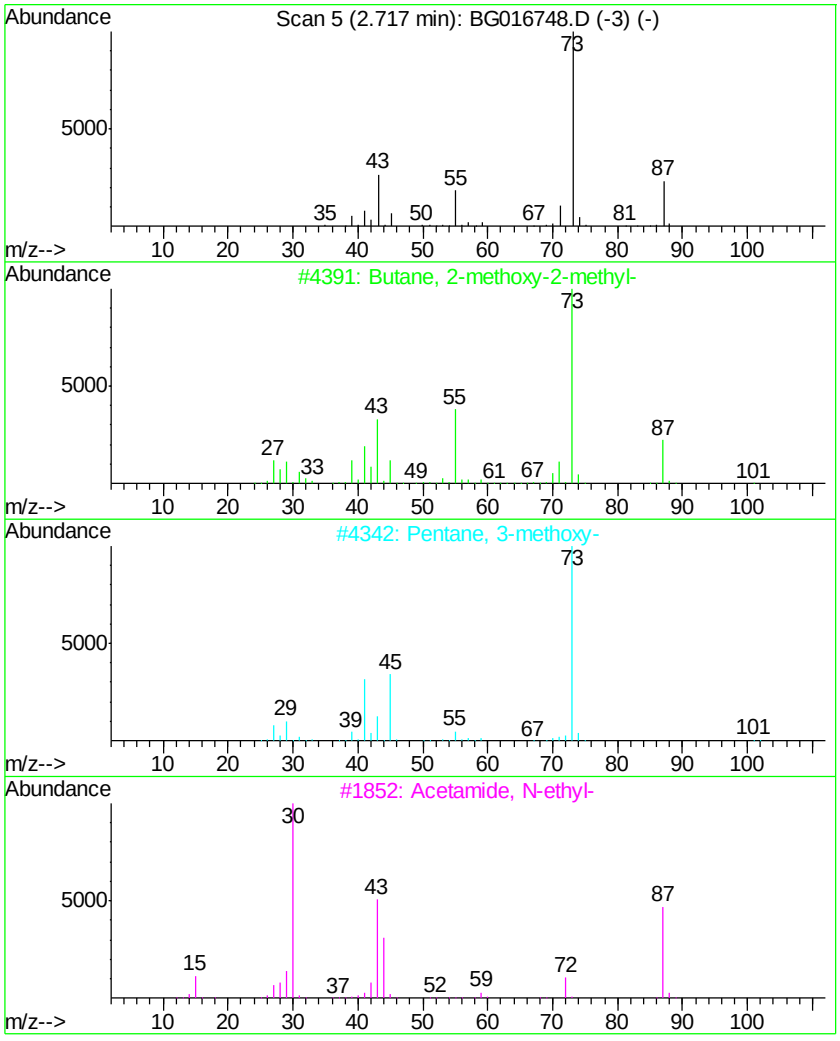
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

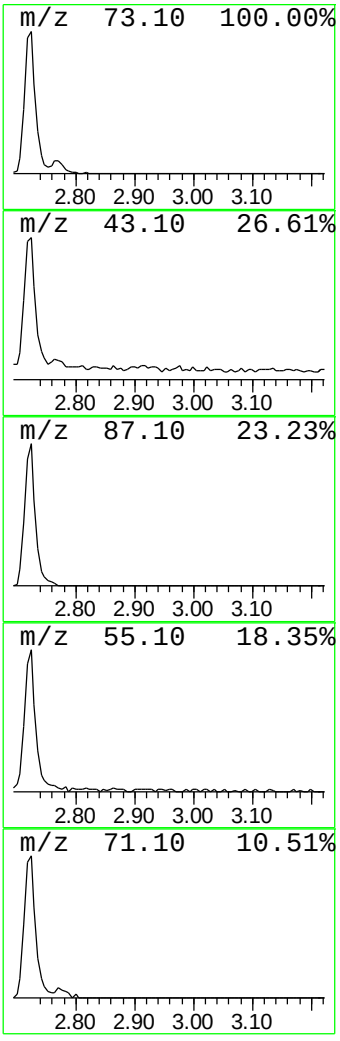
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	7.90 ng	150019	1,4-Dichlorobenzene-d4	7.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

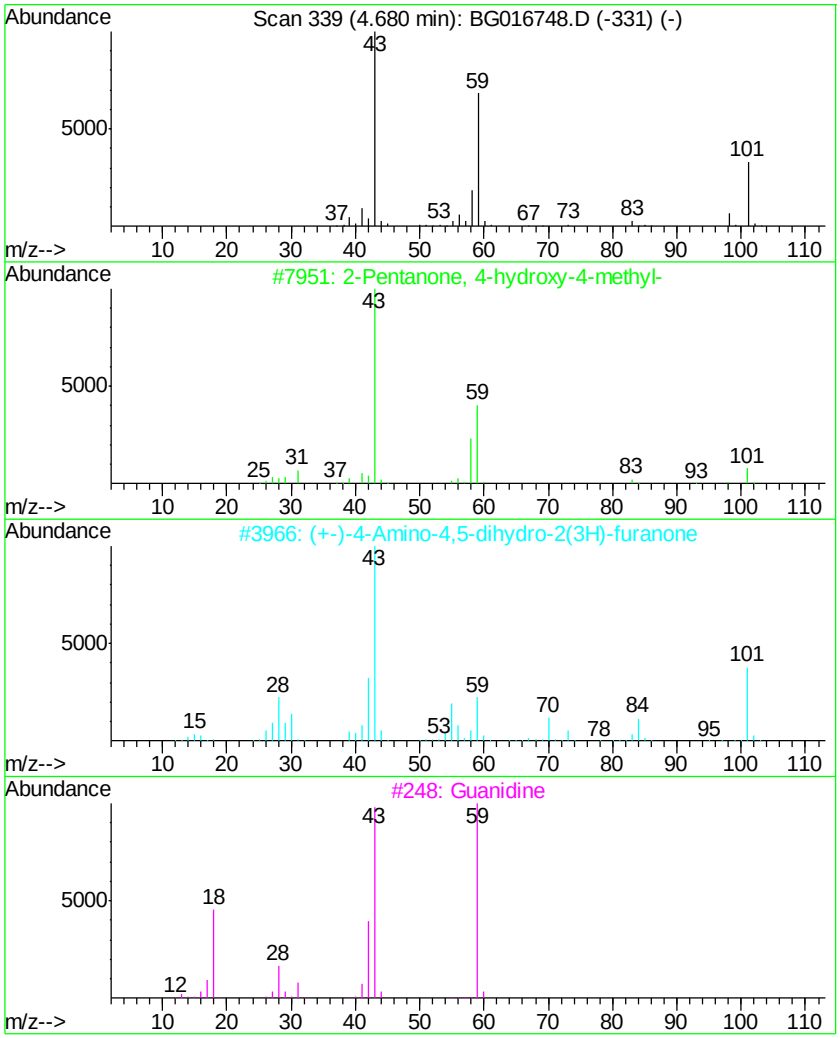
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

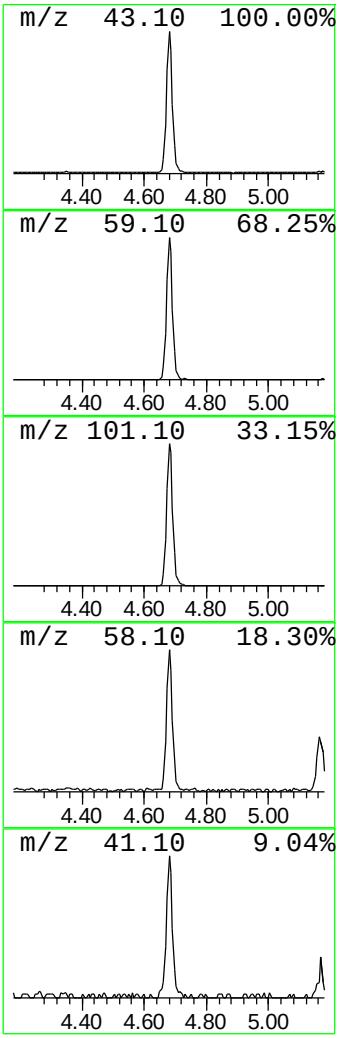
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	14.22 ng	270058	1,4-Dichlorobenzene-d4	7.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Guanidine	59	CH5N3	000113-00-8	43
4	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	23
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17





Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

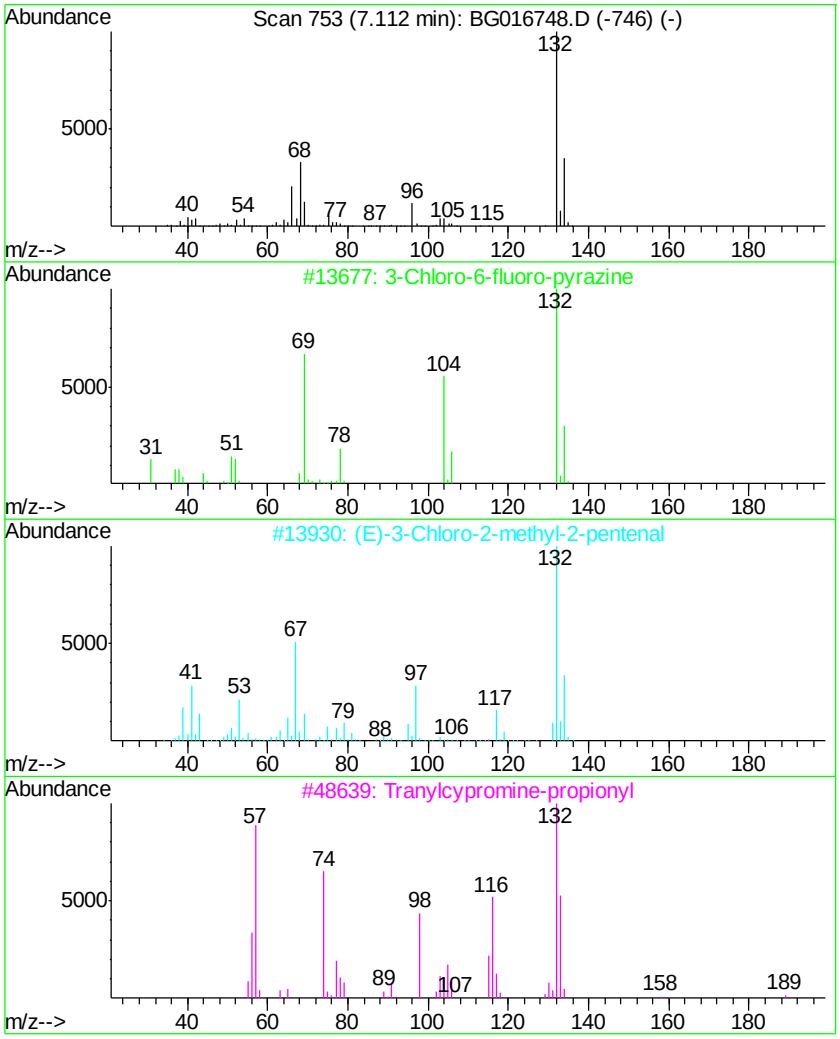
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

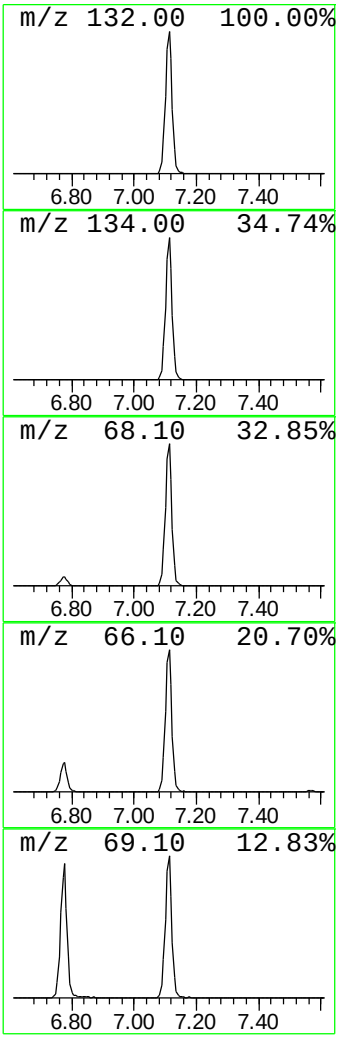
****

Peak Number 3 unknown7.11 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.11	82.08 ng	1559190	1,4-Dichlorobenzene-d4	7.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

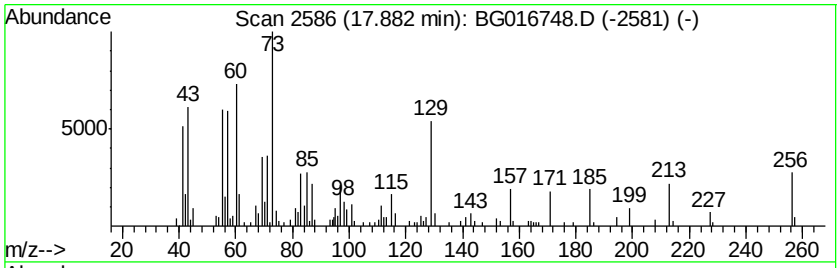
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

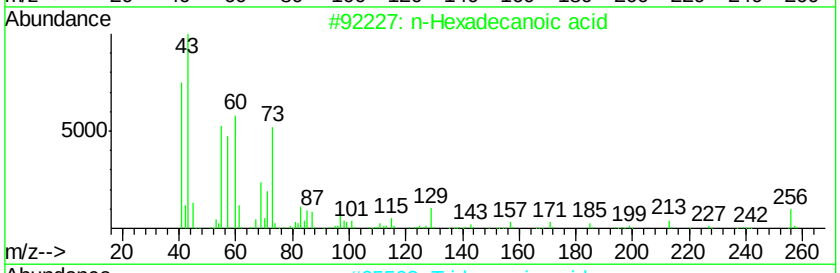
****

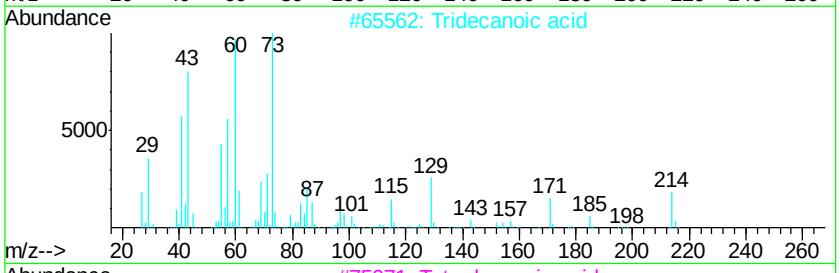
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

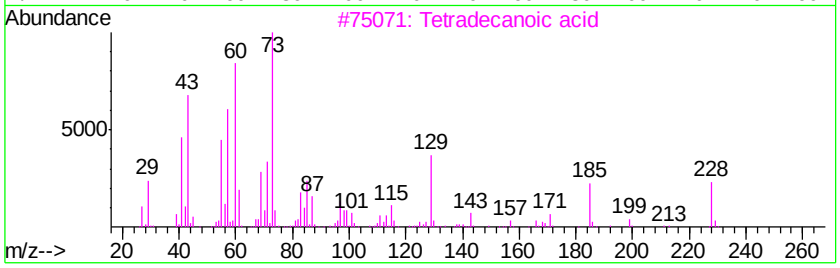
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	4.05 ng	191121	Phenanthrene-d10	16.97

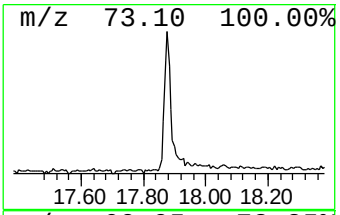
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53

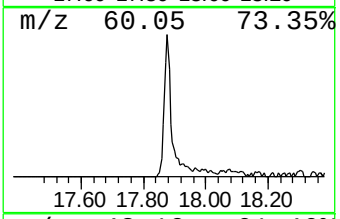


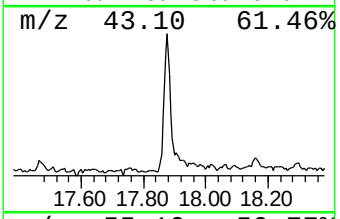


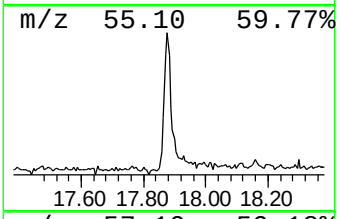


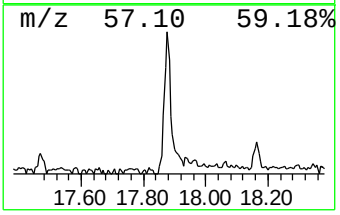












Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

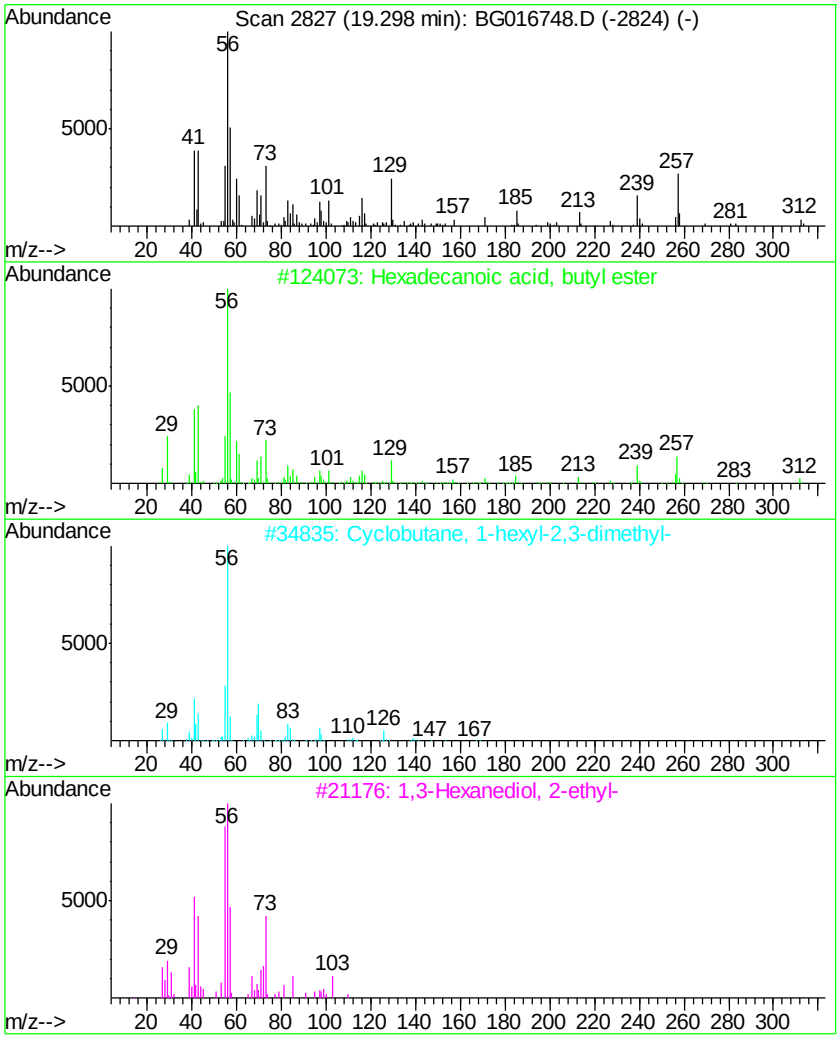
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

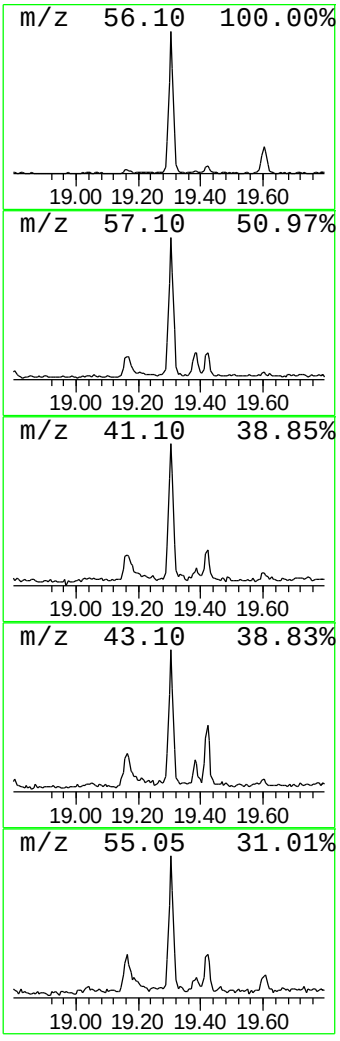
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	3.37 ng	207534	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
3	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	27
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

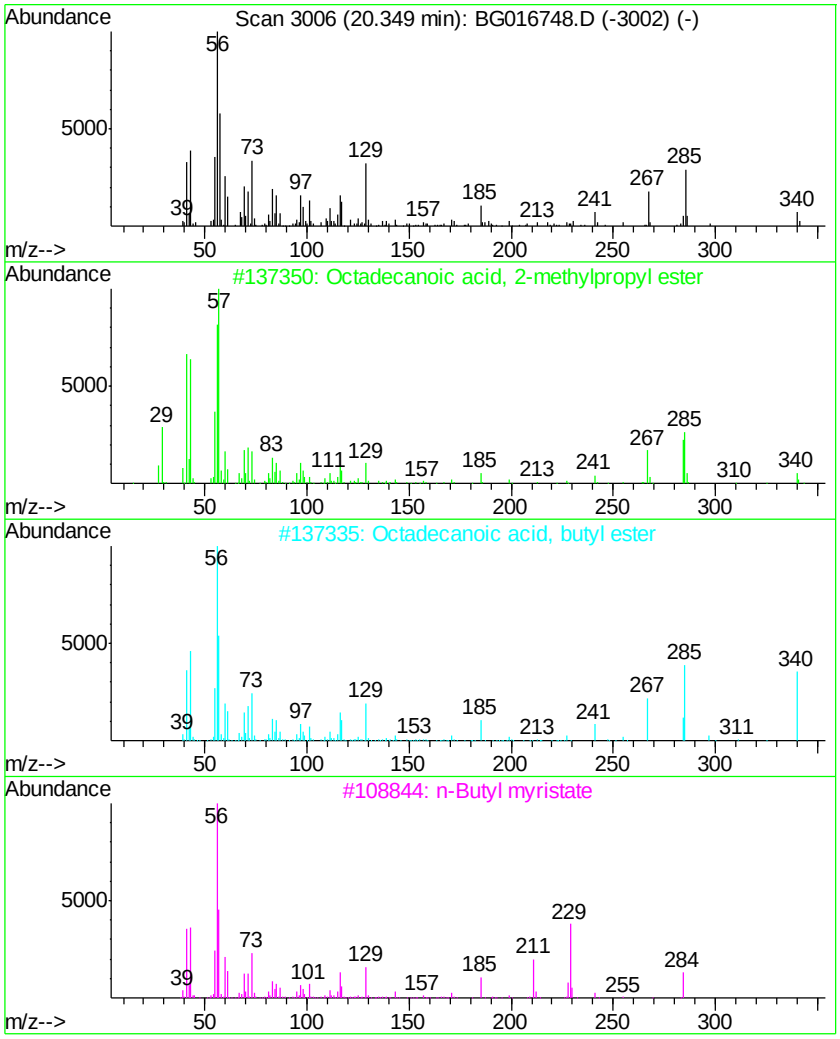
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

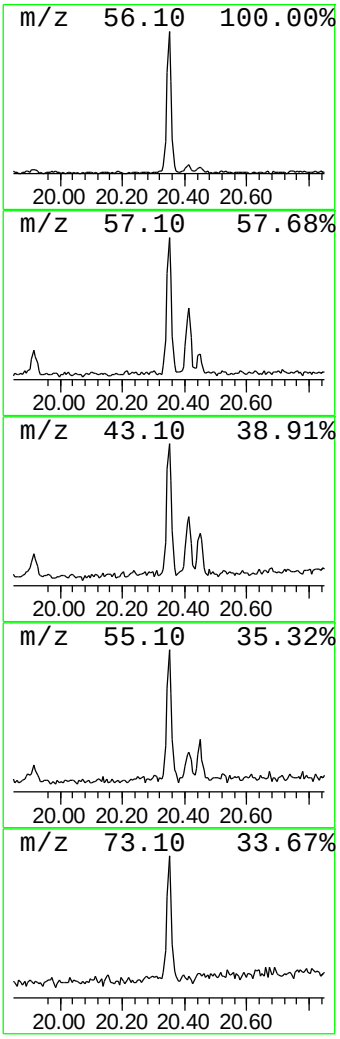
****

Peak Number 7 Octadecanoic acid, 2-methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.35	2.77 ng	170450	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	91
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
3	n-Butyl myristate	284	C18H36O2	000110-36-1	53
4	Propan-2-one O-(2-chloro-1-methy...	149	C6H12ClNO	1000186-05-6	38
5	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	30





Data Path : Z:\HPCHEM1\BNA G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

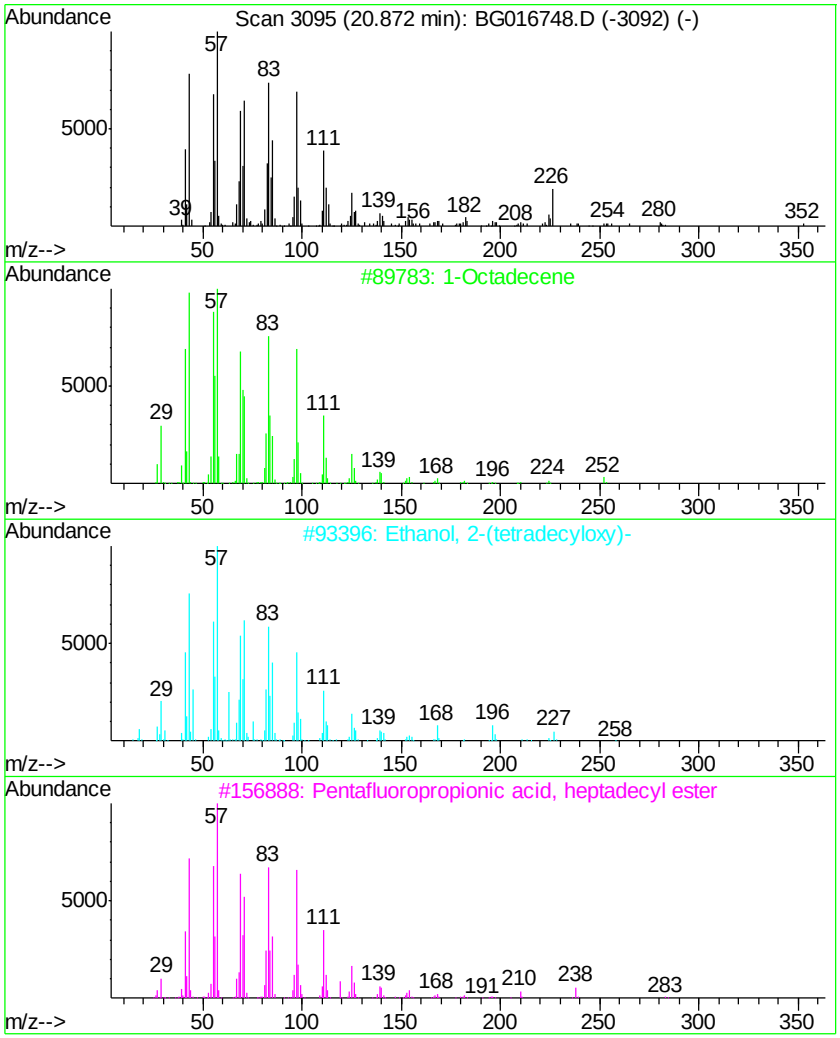
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

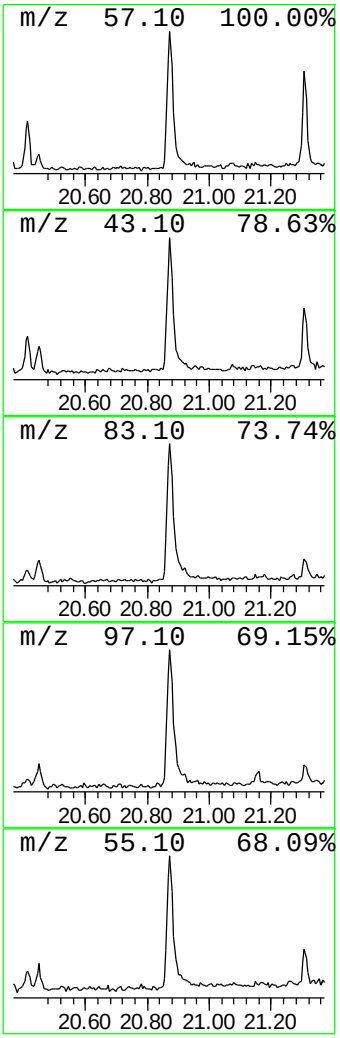
****

Peak Number 8 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	3.32 ng	204841	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	92
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG042715\
Data File : BG016748.D
Acq On : 28 Apr 2015 2:16
Operator : TP/IZ
Sample : G1942-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.72	7.9	ng	150019	1	7.57	379912	20.0
2-Pentanone, 4-hy...	4.68	14.2	ng	270058	1	7.57	379912	20.0
unknown7.11	7.11	82.1	ng	1559190	1	7.57	379912	20.0
n-Hexadecanoic acid	17.88	4.0	ng	191121	4	16.97	943583	20.0
Hexadecanoic acid...	19.30	3.4	ng	207534	5	21.16	1232740	20.0
Octadecanoic acid...	20.35	2.8	ng	170450	5	21.16	1232740	20.0
1-Octadecene	20.87	3.3	ng	204841	5	21.16	1232740	20.0