LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

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-BG120215.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	2.996	21	27	41	rVB	431693	654536	33.81%	5.065%
2	5.187	395	400	409	rVB	96269	143100	7.39%	1.107%
3	5.657	473	480	491	rBV	466538	729293	37.67%	5.644%
4	7.261	744	753	764	rBV	502241	864103	44.63%	6.687%
5	7.643	810	818	832	rBV	474951	804904	41.57%	6.229%
6	8.113	892	898	905	rVB	113100	186720	9.64%	1.445%
7	8.436	946	953	963	rBV	295733	505381	26.10%	3.911%
8	9.277	1088	1096	1106	rBV	295064	529320	27.34%	4.096%
9	10.928	1370	1377	1387	rVB	155306	280357	14.48%	2.170%
10	13.366	1784	1792	1800	rBV	825943	1269672	65.58%	9.826%
11	14.189	1924	1932	1940	rBV	171474	250479	12.94%	1.938%
12	14.623	2001	2006	2011	rBV2	25665	34685	1.79%	0.268%
13	14.741	2020	2026	2038	rVB2	271662	436617	22.55%	3.379%
14	15.575	2163	2168	2172	rVB	38160	49820	2.57%	0.386%
15	15.981	2229	2237	2241	rBV3	12041	24374	1.26%	0.189%
16	16.221	2270	2278	2288	rBV	702043	1044054	53.93%	8.080%
17	16.433	2310	2314	2317	rBV	39966	51366	2.65%	0.398%
18	16.862	2384	2387	2395	rVB6	8791	19768	1.02%	0.153%
19	17.226	2443	2449	2452	rBV	25300	31333	1.62%	0.242%
20	17.485	2486	2493	2499	rBV	378564	570190	29.45%	4.413%
21	18.354	2636	2641	2648	rBV	92655	137519	7.10%	1.064%
22	18.877	2725	2730	2735	rBV2	15038	22027	1.14%	0.170%
23	19.212	2783	2787	2792	rBV2	30018	40260	2.08%	0.312%
24	19.623	2853	2857	2866	rBV2	37449	57683	2.98%	0.446%
25	19.770	2875	2882	2888	rBV2	55273	100071	5.17%	0.774%
26	19.888	2899	2902	2906	rVB3	21123	24424	1.26%	0.189%
27	20.082	2930	2935	2941	rBV	1460177	1936045	100.00%	14.983%
28	20.287	2966	2970	2974	rVB3	23332	30932	1.60%	0.239%
29	20.763	3047	3051	3056	rVB	38626	49915	2.58%	0.386%
30	20.816	3056	3060	3062	rBV2	45371	55448	2.86%	0.429%
31	20.981	3084	3088	3093	rVV3	24503	45665	2.36%	0.353%
32	21.028	3093	3096	3100	rVV	39985	52812	2.73%	0.409%
33	21.098	3104	3108	3115	rVB2	21768	32863	1.70%	0.254%
34	21.386	3153	3157	3165	rVB2	112844	167753	8.66%	1.298%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.539	3175	3183	3189	rBV2	32308	61236	3.16%	0.474%
36	21.639	3196	3200	3205	rVB	44933	67919	3.51%	0.526%
37	21.756	3213	3220	3227	rVB	447127	741816	38.32%	5.741%
38	21.950	3249	3253	3258	rVB2	23569	33365	1.72%	0.258%
39	22.567	3355	3358	3367	rBV7	13311	26328	1.36%	0.204%
40	23.278	3475	3479	3484	rVB5	12195	21531	1.11%	0.167%
41	23.478	3508	3513	3518	rBV3	19881	35563	1.84%	0.275%
42	25.035	3768	3778	3791	rBV	241412	700502	36.18%	5.421%

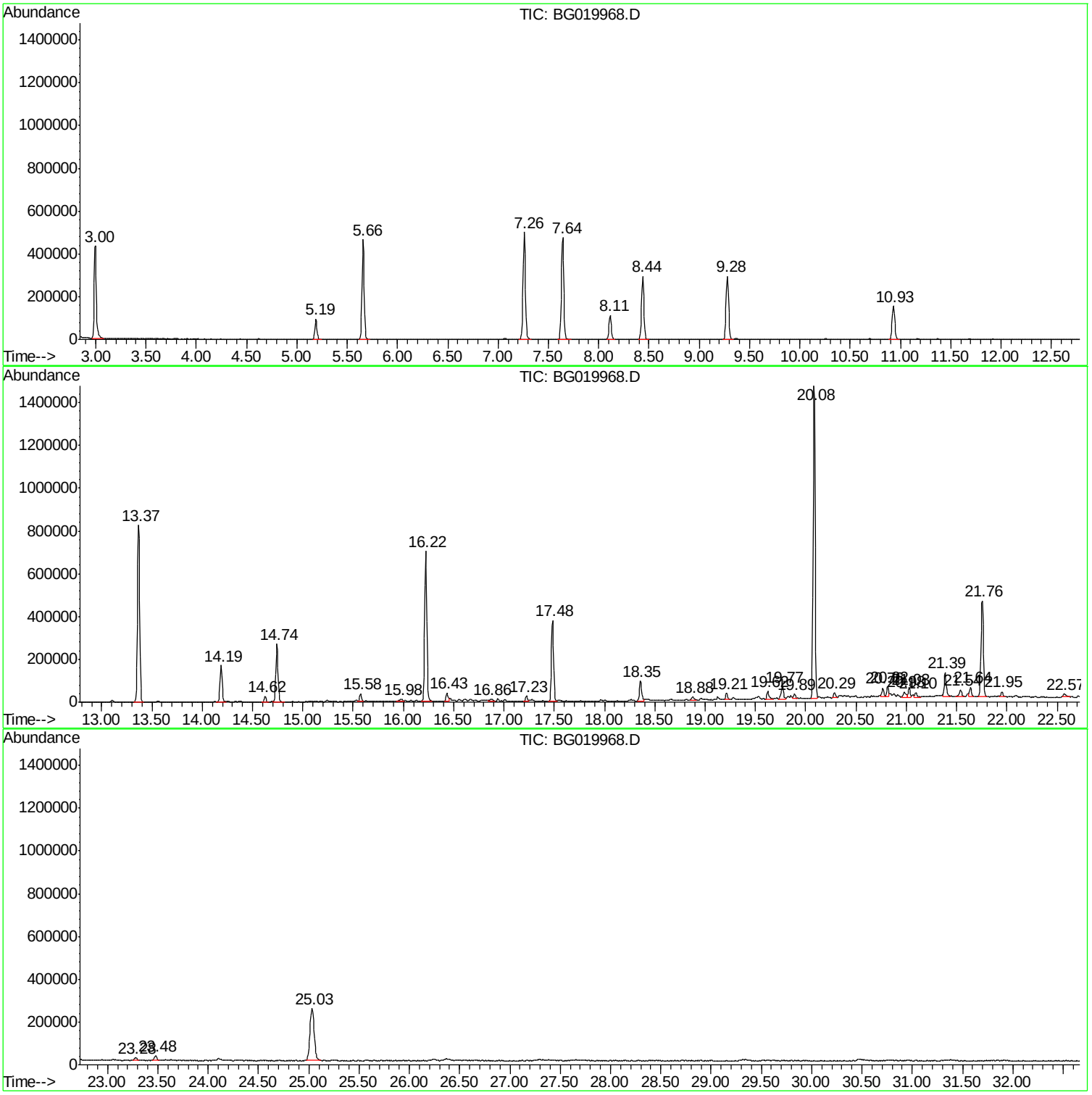
Sum of corrected areas: 12921749

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

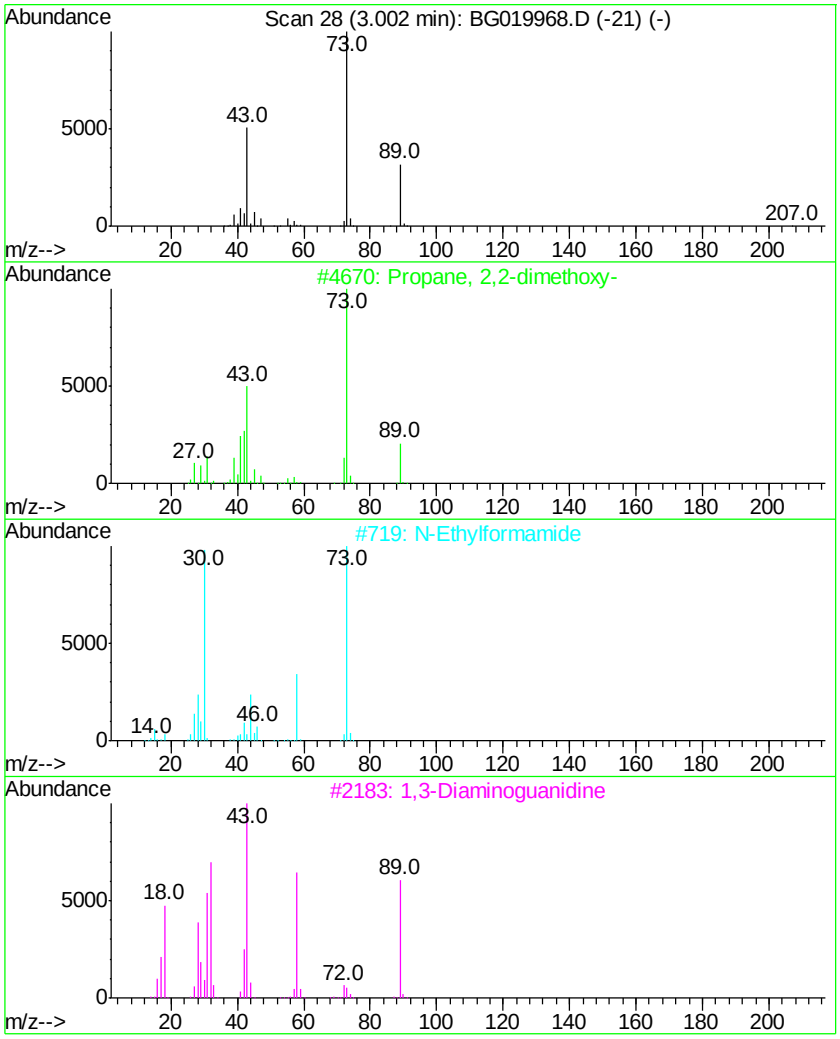
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

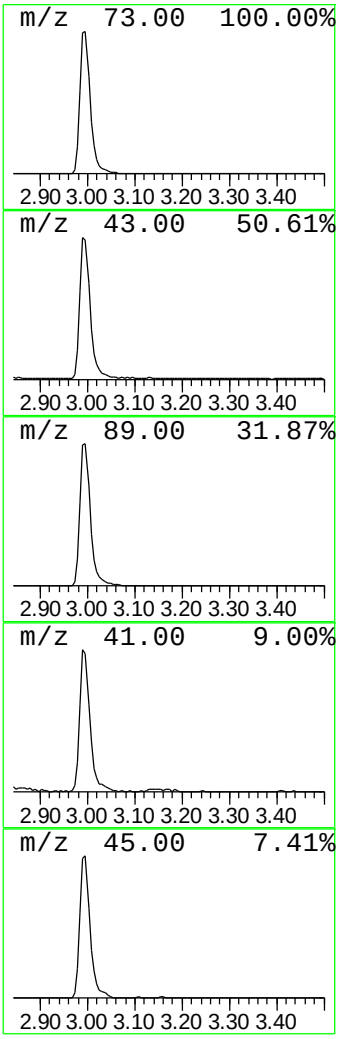
****

Peak Number 1 unknown3.00 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	70.11 ng	654536	1,4-Dichlorobenzene-d4	8.11

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	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

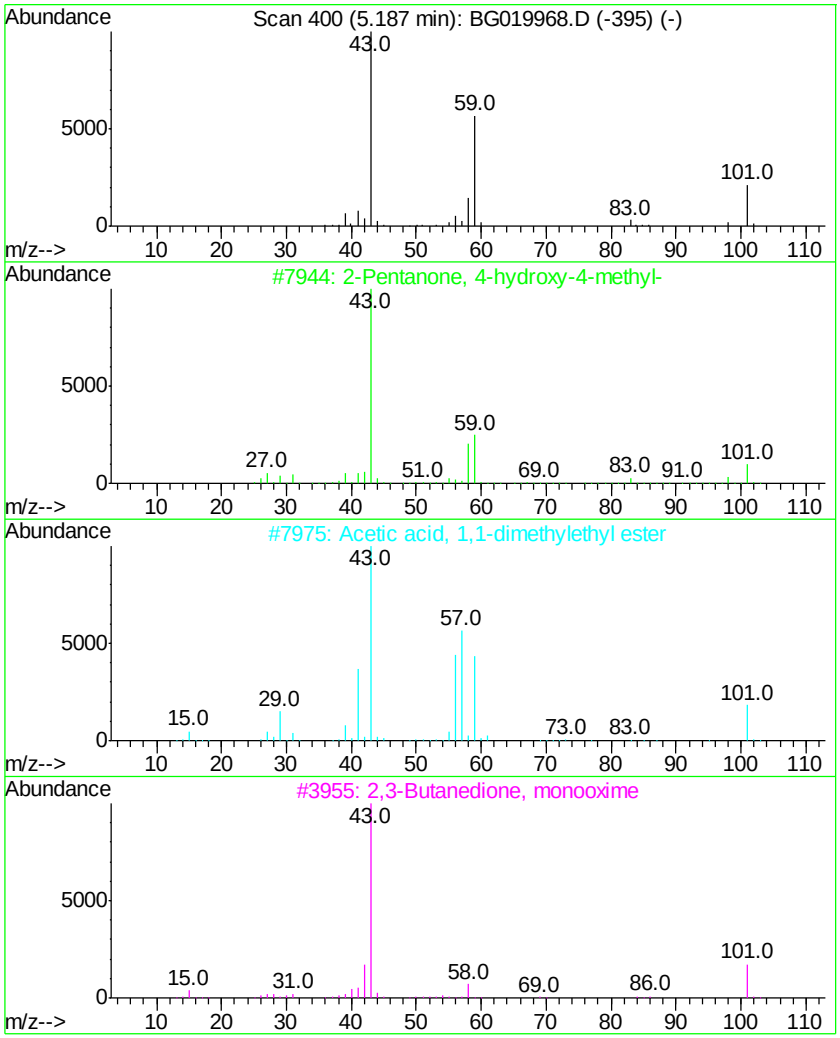
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

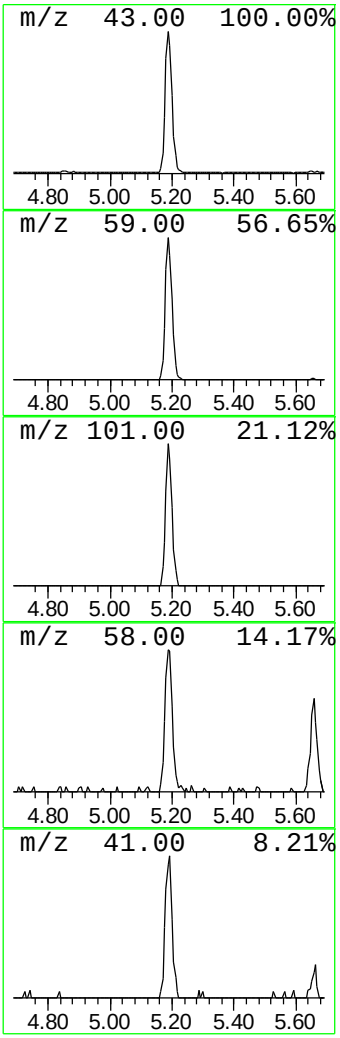
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	15.33 ng	143100	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

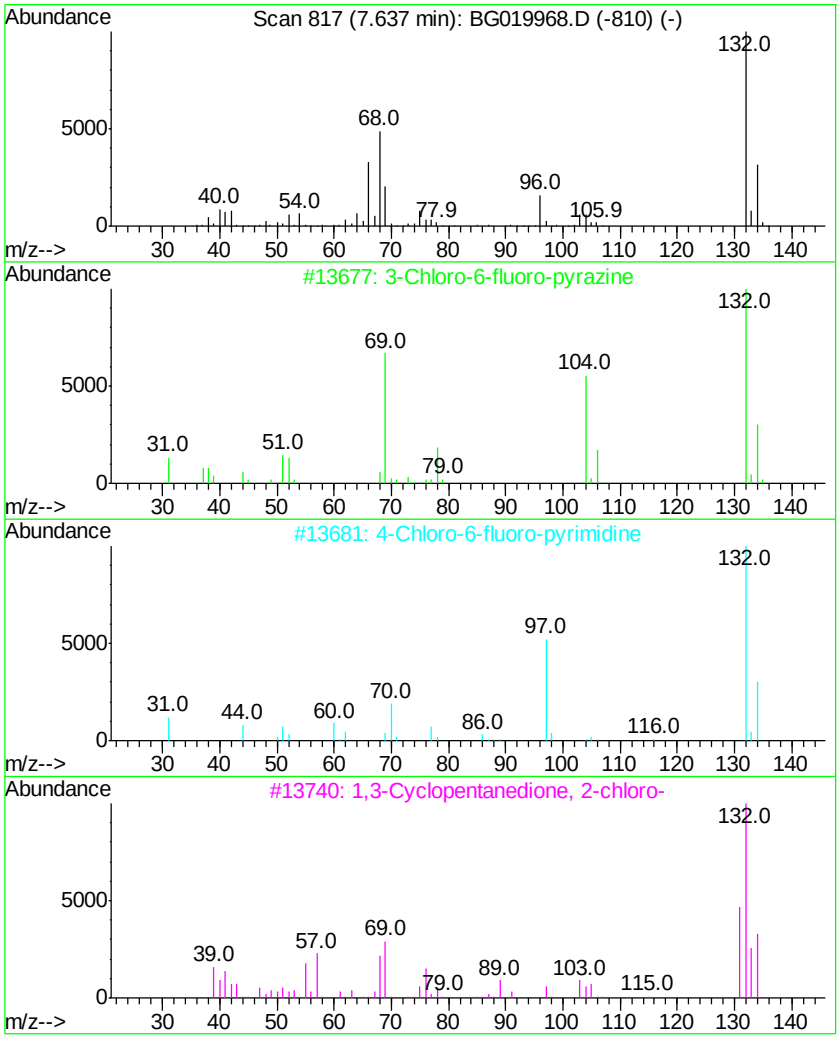
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

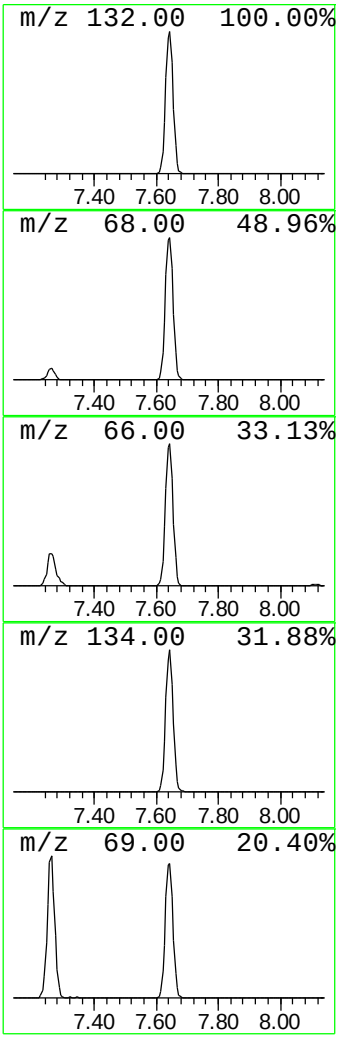
****

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	86.22 ng	804904	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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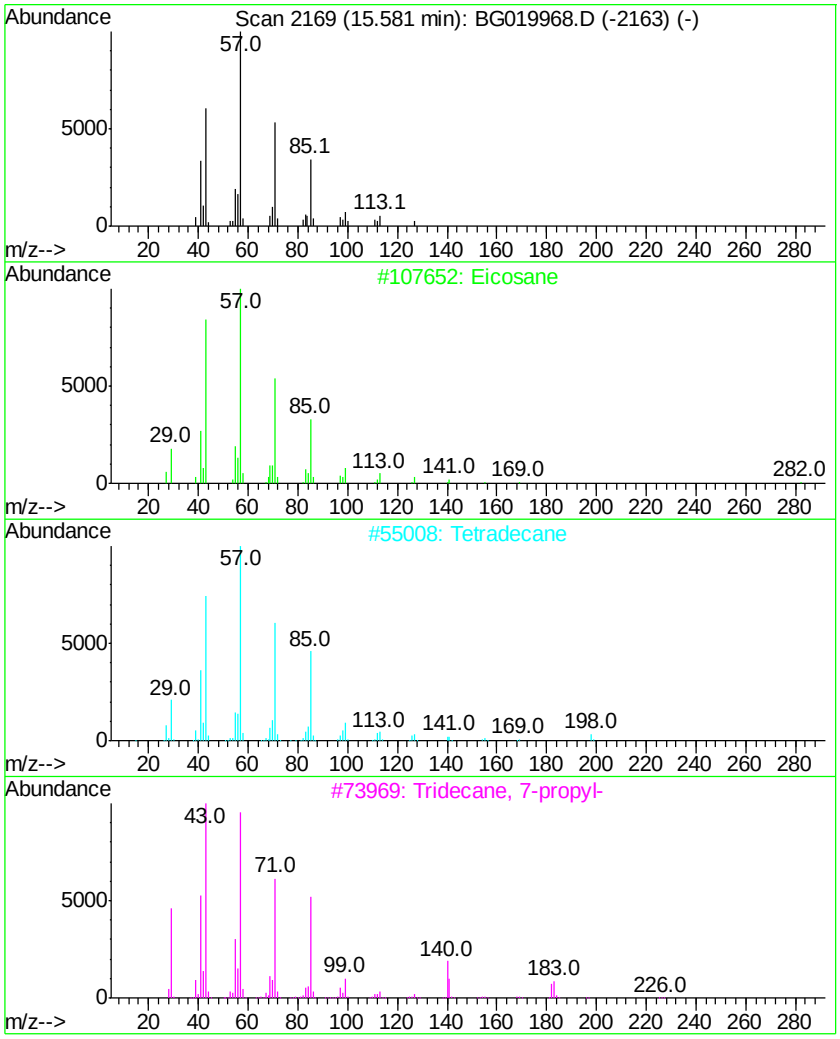
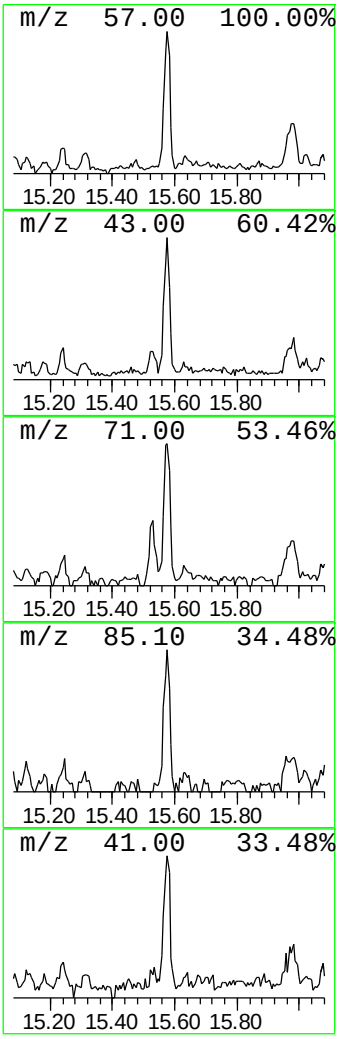
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.28 ng	49820	Acenaphthene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

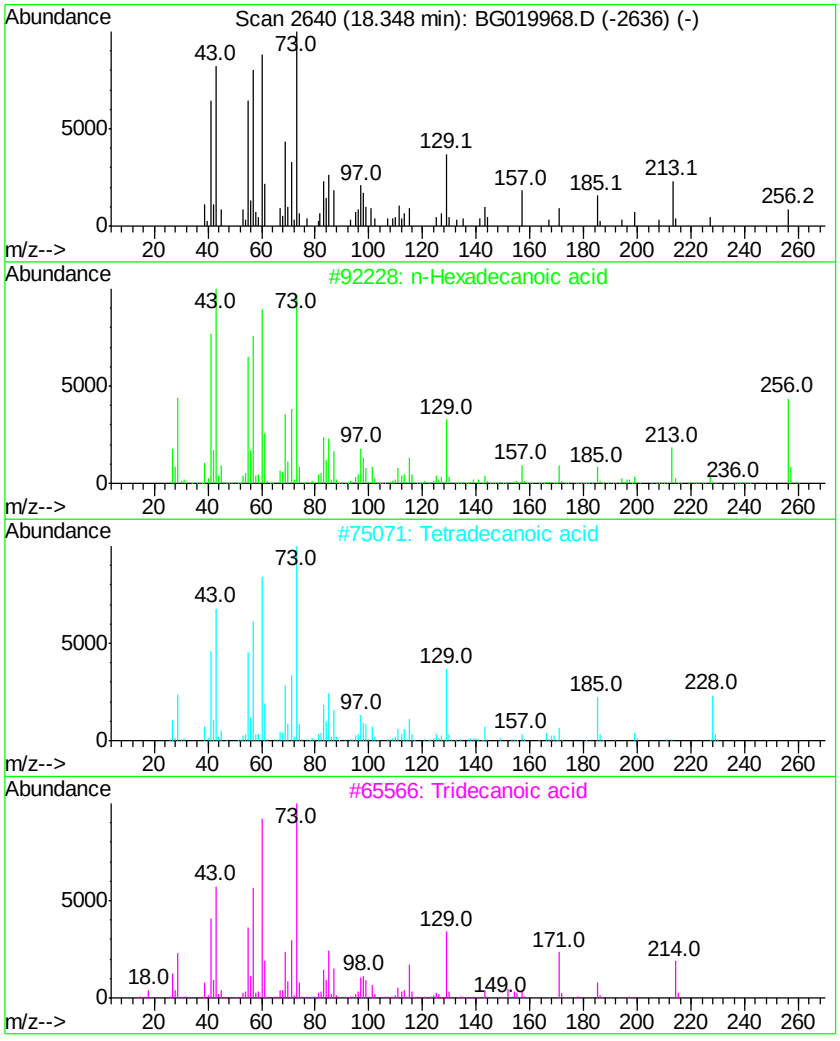
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

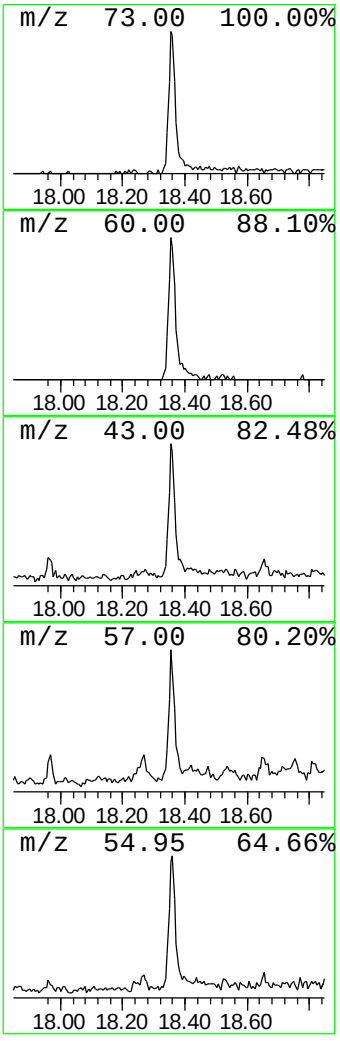
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	4.82 ng	137519	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

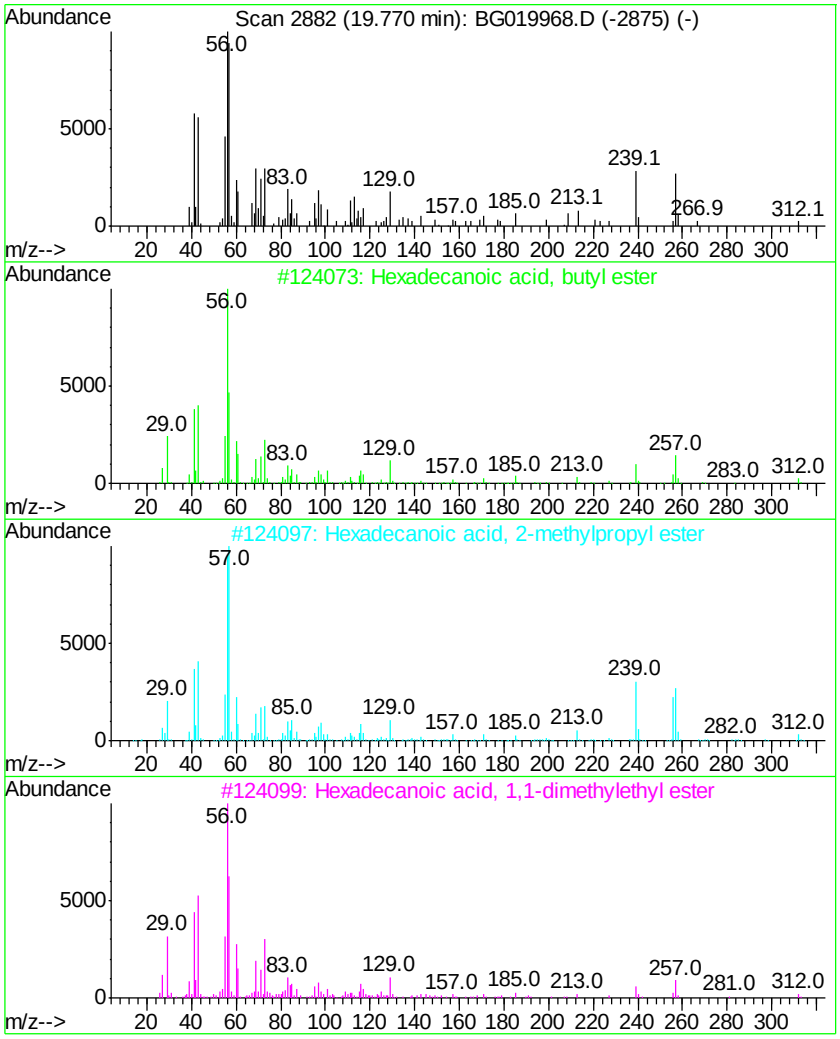
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

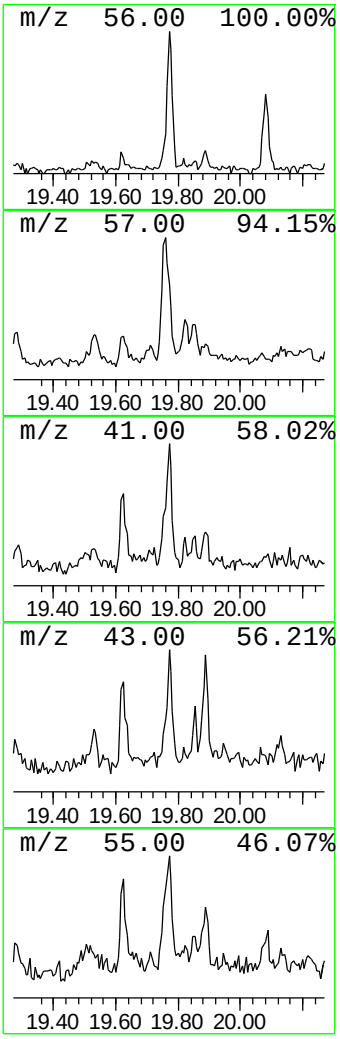
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.70 ng	100071	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	93
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	93
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	76
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30
5	Cycloheptylamine	113	C7H15N	005452-35-7	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

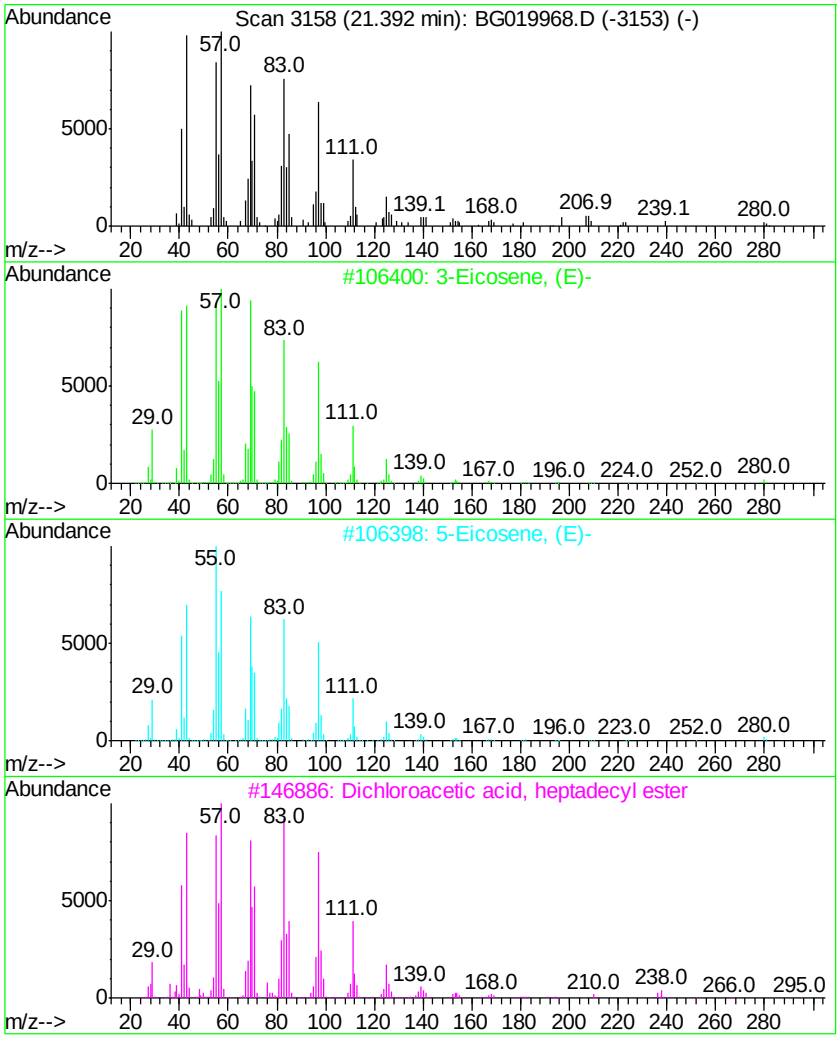
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

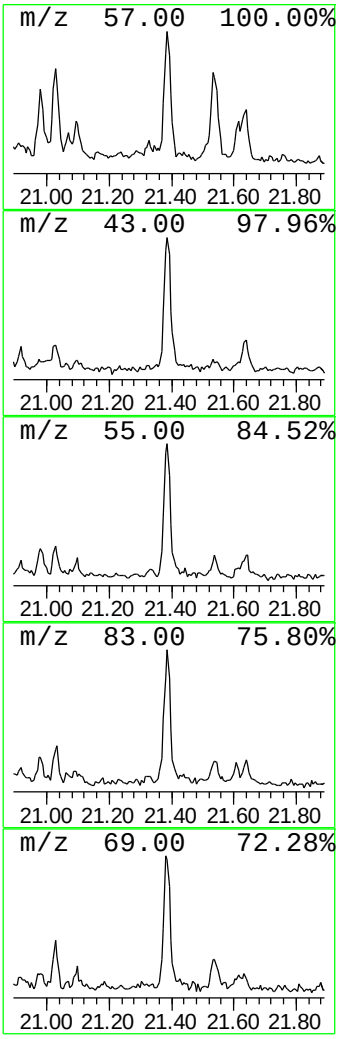
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	4.52 ng	167753	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	1-Eicosene	280	C20H40	003452-07-1	93
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019968.D
Acq On : 6 Dec 2015 15:45
Operator : UM/NP
Sample : G4650-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COFF(0-2)-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
unknown3.00	3.00	70.1	ng	654536	1	8.11	186720	20.0
2-Pentanone, 4-hy...	5.19	15.3	ng	143100	1	8.11	186720	20.0
unknown7.64	7.64	86.2	ng	804904	1	8.11	186720	20.0
Eicosane	15.58	2.3	ng	49820	3	14.74	436617	20.0
n-Hexadecanoic acid	18.35	4.8	ng	137519	4	17.48	570190	20.0
Hexadecanoic acid...	19.77	2.7	ng	100071	5	21.76	741816	20.0
3-Eicosene, (E)-	21.39	4.5	ng	167753	5	21.76	741816	20.0