LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016914.D
Acq On : 7 May 2015 9:39
Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

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-BG050515.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	2.782	12	16	35	rBV	5547467	7403038	100.00%	22.303%
2	2.917	35	39	48	rVB2	168809	307684	4.16%	0.927%
3	3.000	49	53	58	rVB	173262	197388	2.67%	0.595%
4	4.915	374	379	387	rBV	182681	254465	3.44%	0.767%
5	5.373	450	457	468	rVB	1352071	2010037	27.15%	6.056%
6	6.960	719	727	736	rBV	1467125	2275234	30.73%	6.855%
7	7.330	782	790	802	rVB	1314906	2151253	29.06%	6.481%
8	7.794	863	869	876	rVB	289887	455705	6.16%	1.373%
9	8.117	916	924	931	rBV	853817	1378901	18.63%	4.154%
10	8.952	1054	1066	1075	rBV	826261	1334634	18.03%	4.021%
11	10.591	1338	1345	1352	rVB	400057	650964	8.79%	1.961%
12	13.058	1757	1765	1771	rBV	1760880	2516183	33.99%	7.580%
13	13.893	1902	1907	1911	rBV	85772	114701	1.55%	0.346%
14	14.433	1993	1999	2006	rBV2	564587	918673	12.41%	2.768%
15	15.926	2244	2253	2262	rBV	1617215	2362071	31.91%	7.116%
16	17.177	2460	2466	2471	rBV2	785430	1165619	15.75%	3.512%
17	18.076	2613	2619	2629	rBV2	149938	242932	3.28%	0.732%
18	19.239	2807	2817	2824	rBV	98238	171099	2.31%	0.515%
19	19.357	2833	2837	2845	rBV3	85742	117924	1.59%	0.355%
20	19.598	2868	2878	2881	rBV2	71337	121980	1.65%	0.367%
21	19.809	2906	2914	2923	rVB	2933600	3659720	49.44%	11.026%
22	20.503	3025	3032	3037	rBV	127744	276657	3.74%	0.833%
23	20.550	3037	3040	3047	rVB5	79333	131933	1.78%	0.397%
24	21.078	3126	3130	3137	rBV	184190	253936	3.43%	0.765%
25	21.360	3171	3178	3182	rBV	1035271	1343491	18.15%	4.048%
26	22.970	3447	3452	3455	rBV5	44423	74187	1.00%	0.224%
27	23.564	3548	3553	3558	rBV4	42349	78784	1.06%	0.237%
28	23.664	3563	3570	3580	rBV2	629293	1223752	16.53%	3.687%

Sum of corrected areas: 33192945

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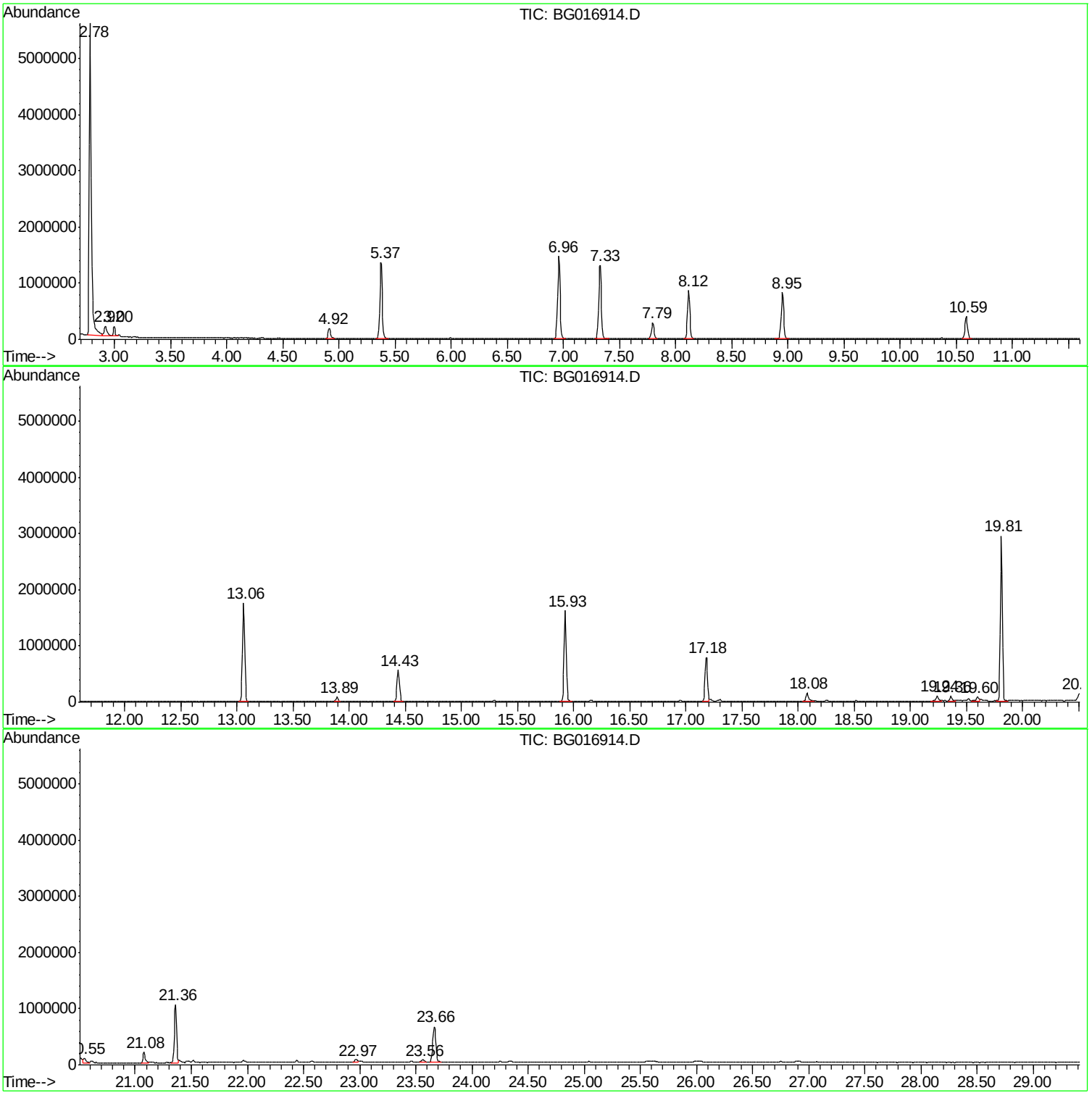
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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\BG050715\
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Operator : TP/IZ
Sample : G2044-16
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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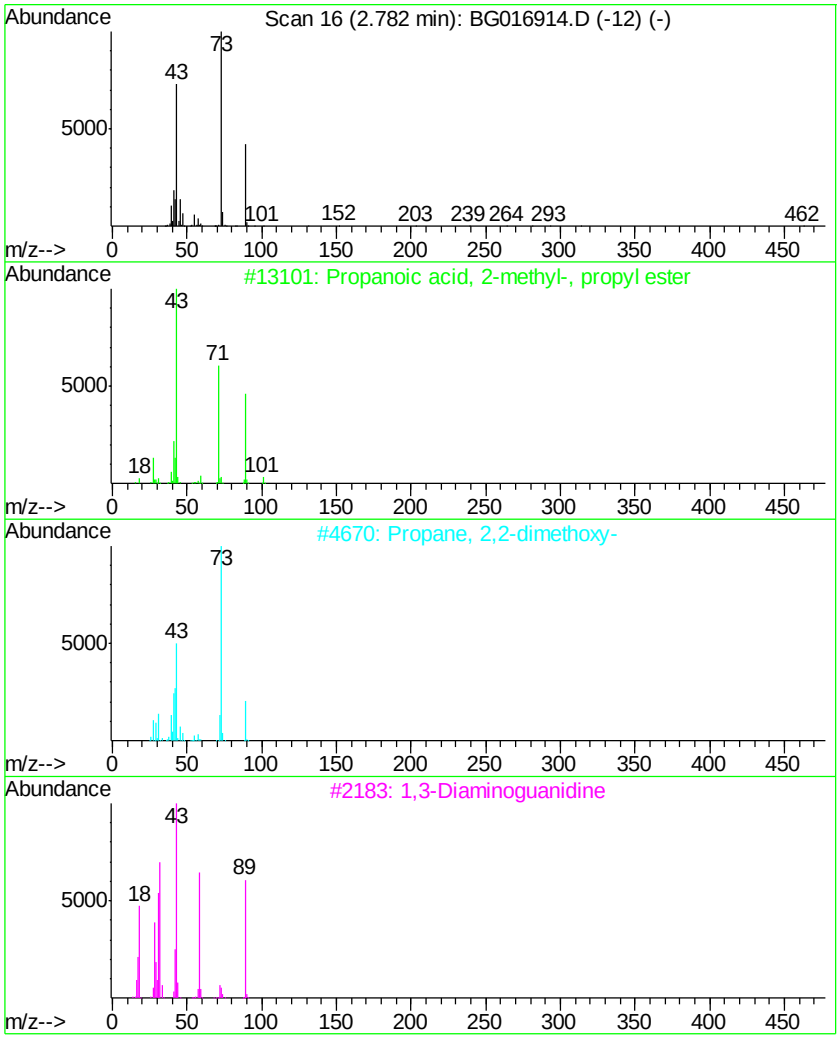
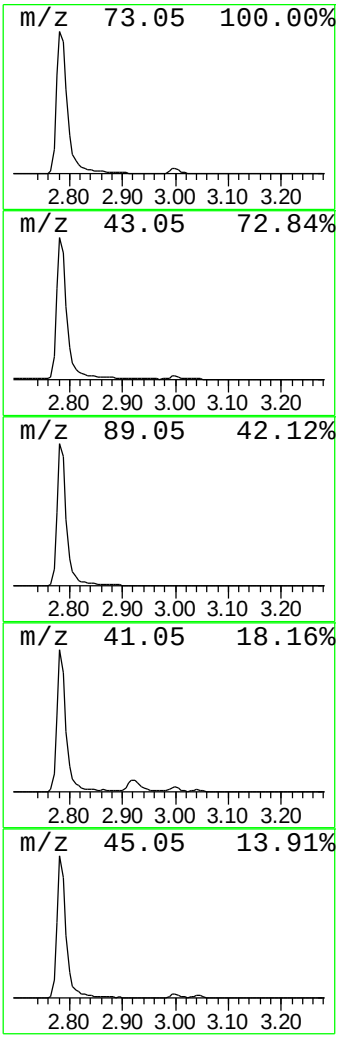
Peak Number 1 unknown2.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.78	324.91 ng	7403040	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	38
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016914.D
Acq On : 7 May 2015 9:39
Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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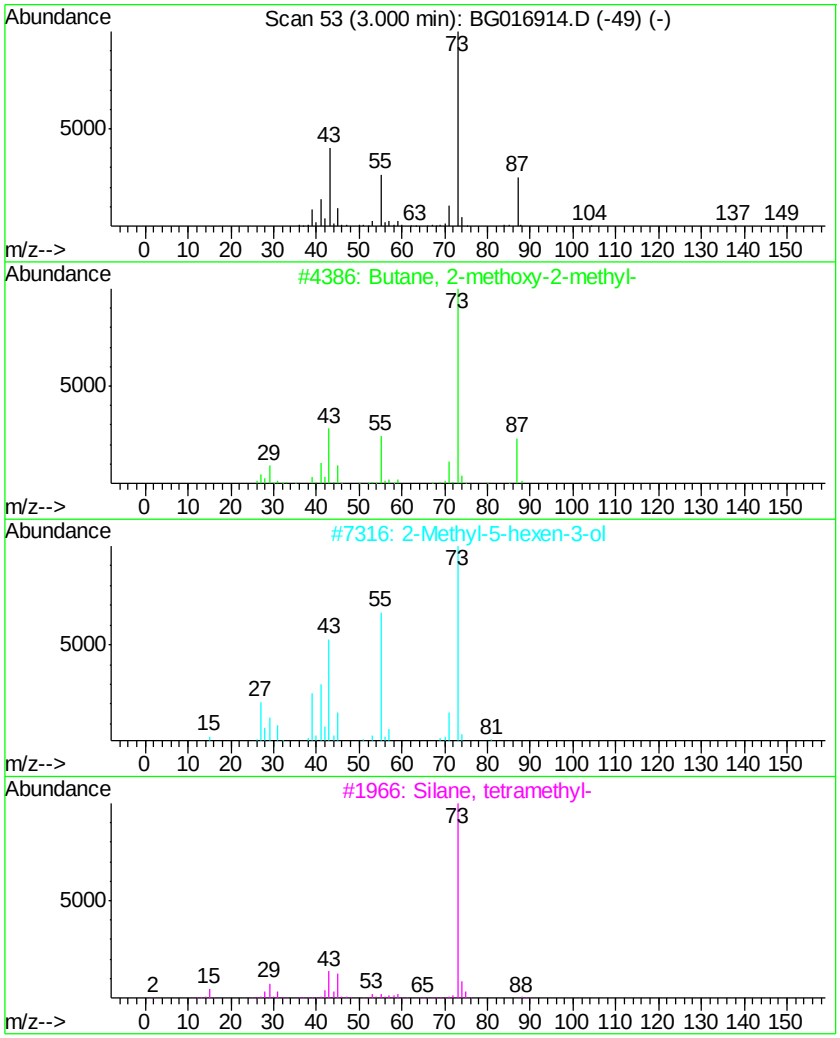
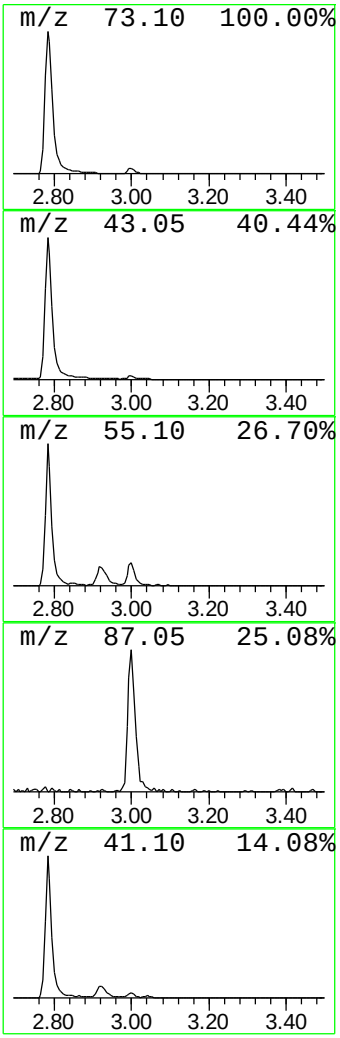
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	8.66 ng	197388	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
4	Epi-Inositol	180	C6H12O6	000488-58-4	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016914.D
Acq On : 7 May 2015 9:39
Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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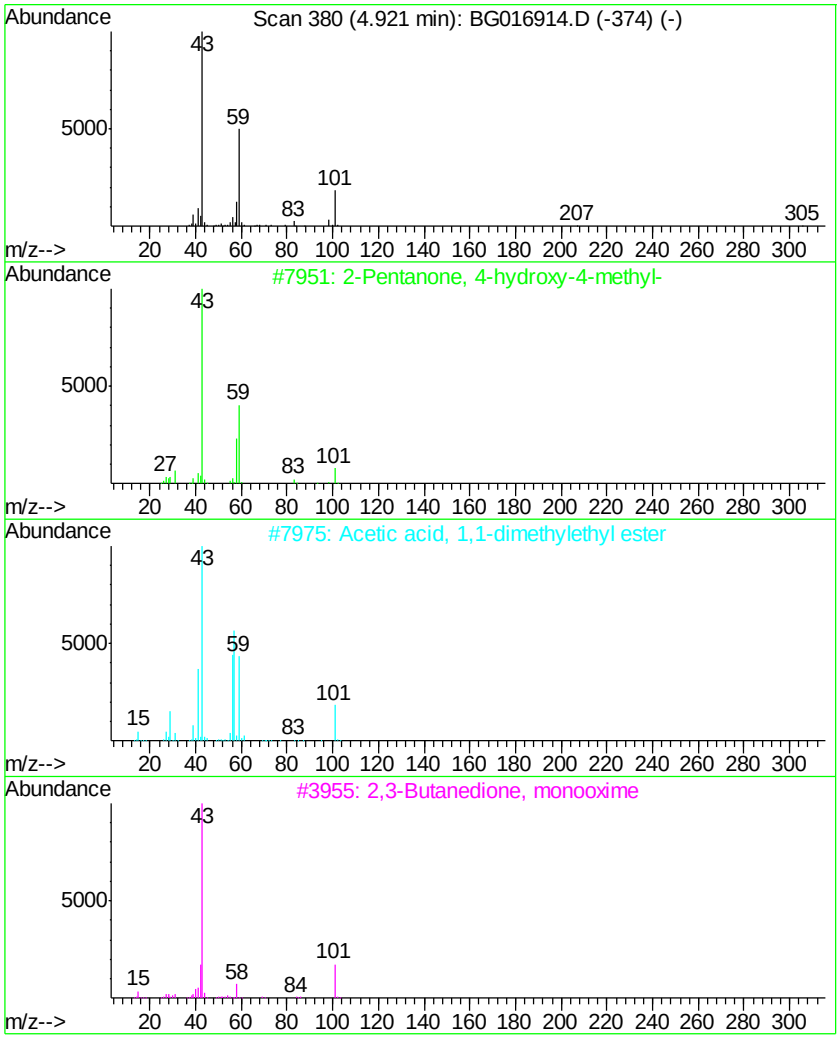
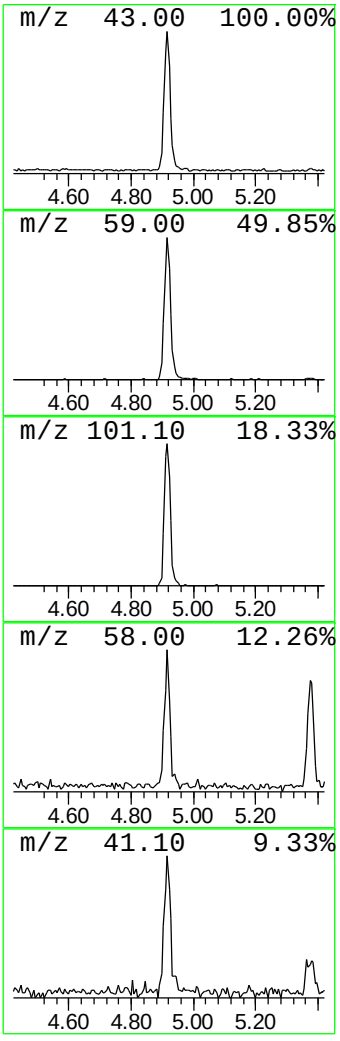
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	11.17 ng	254465	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016914.D
Acq On : 7 May 2015 9:39
Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

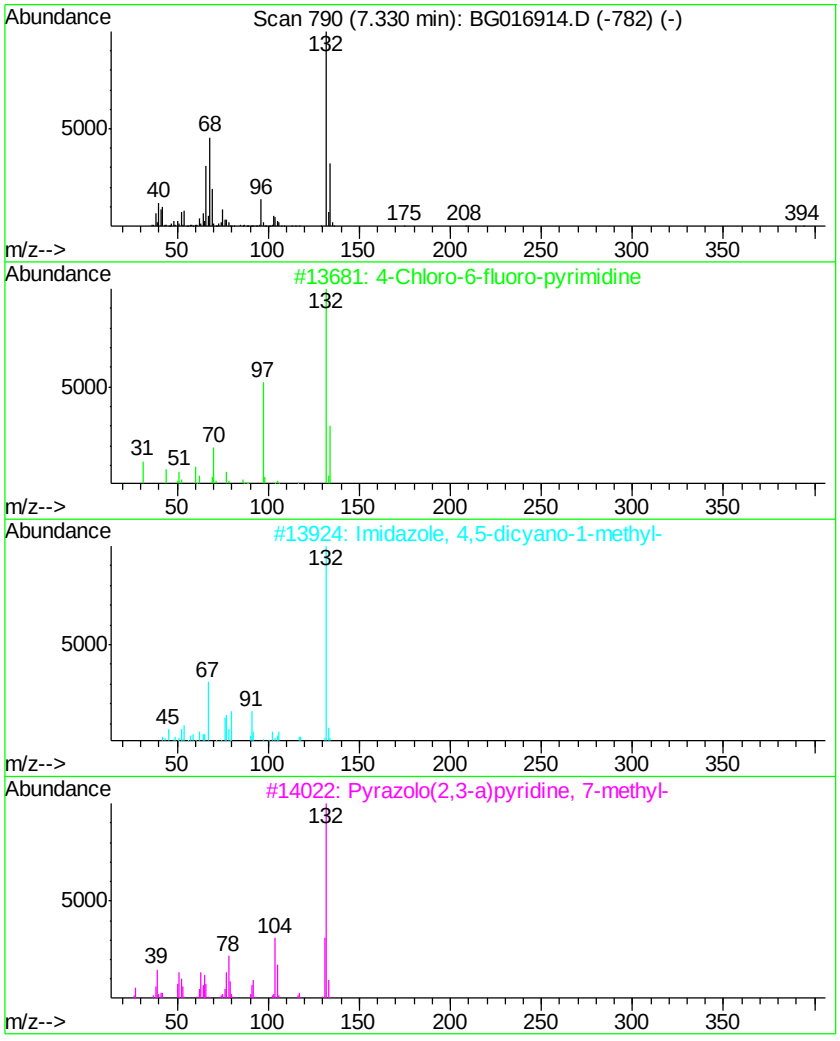
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

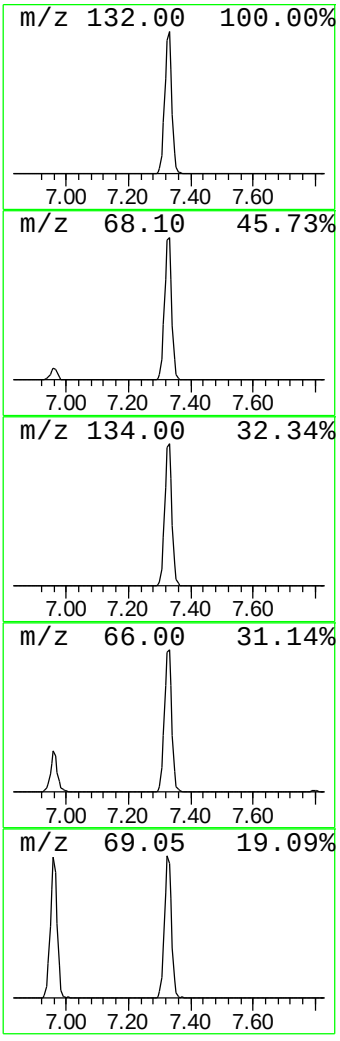
****

Peak Number 5 unknown7.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	94.41 ng	2151250	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016914.D
Acq On : 7 May 2015 9:39
Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

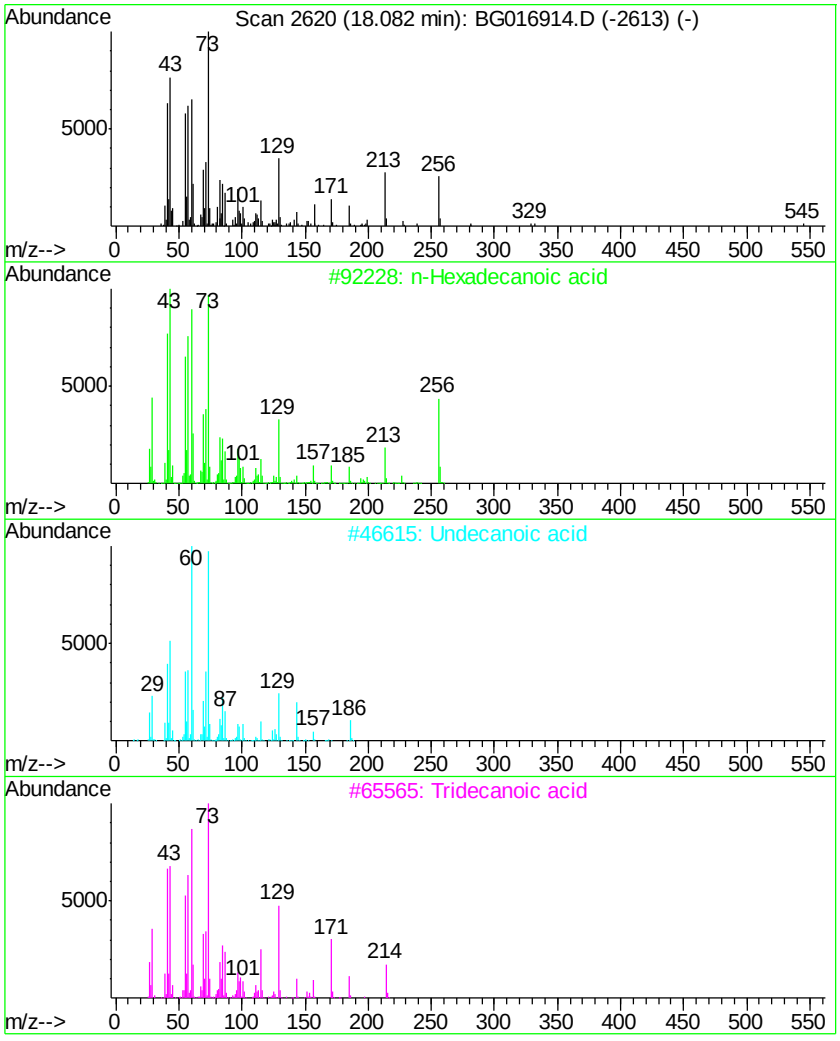
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

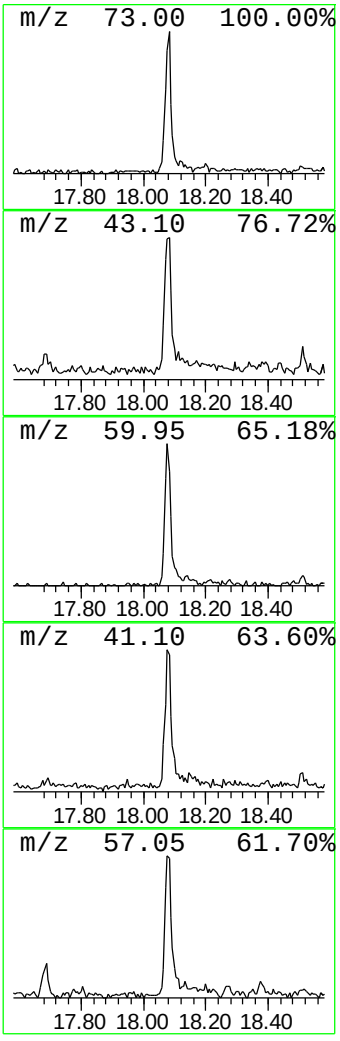
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	4.17 ng	242932	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Undecanoic acid	186	C11H22O2	000112-37-8	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





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Operator : TP/IZ
Sample : G2044-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

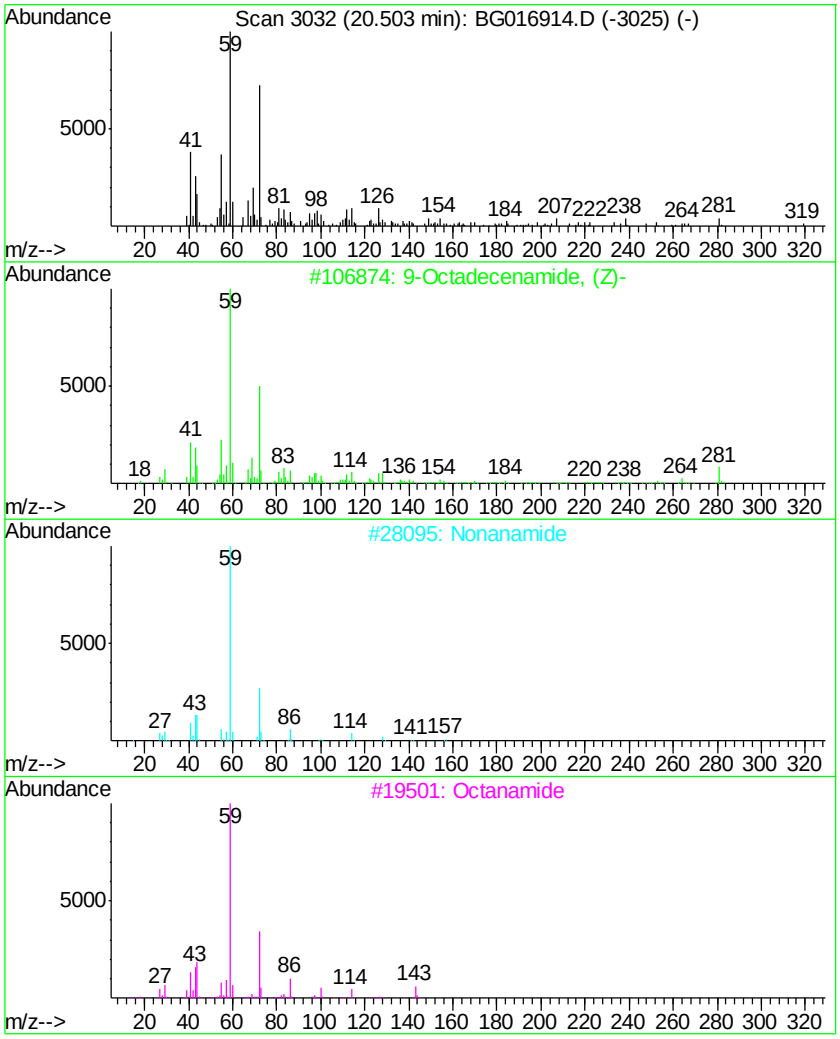
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

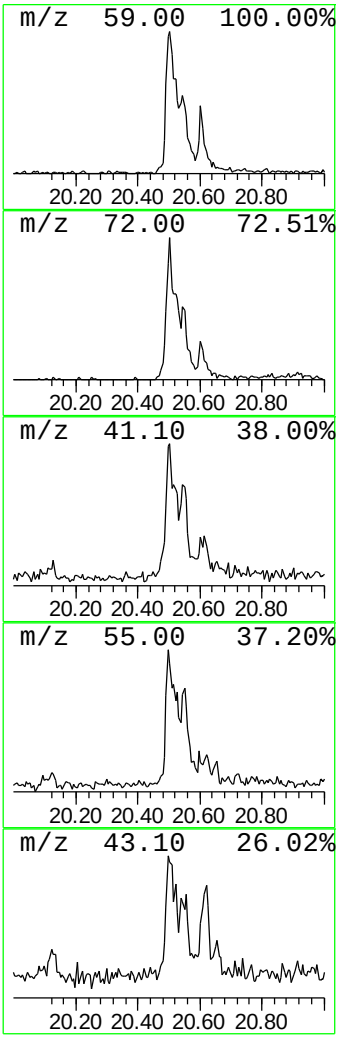
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.50	4.12 ng	276657	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Nonanamide	157	C9H19NO	001120-07-6	52
3	Octanamide	143	C8H17NO	000629-01-6	50
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
5	Cyclooctanemethanol, .alpha.,.al...	170	C11H22O	016624-06-9	38





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-48D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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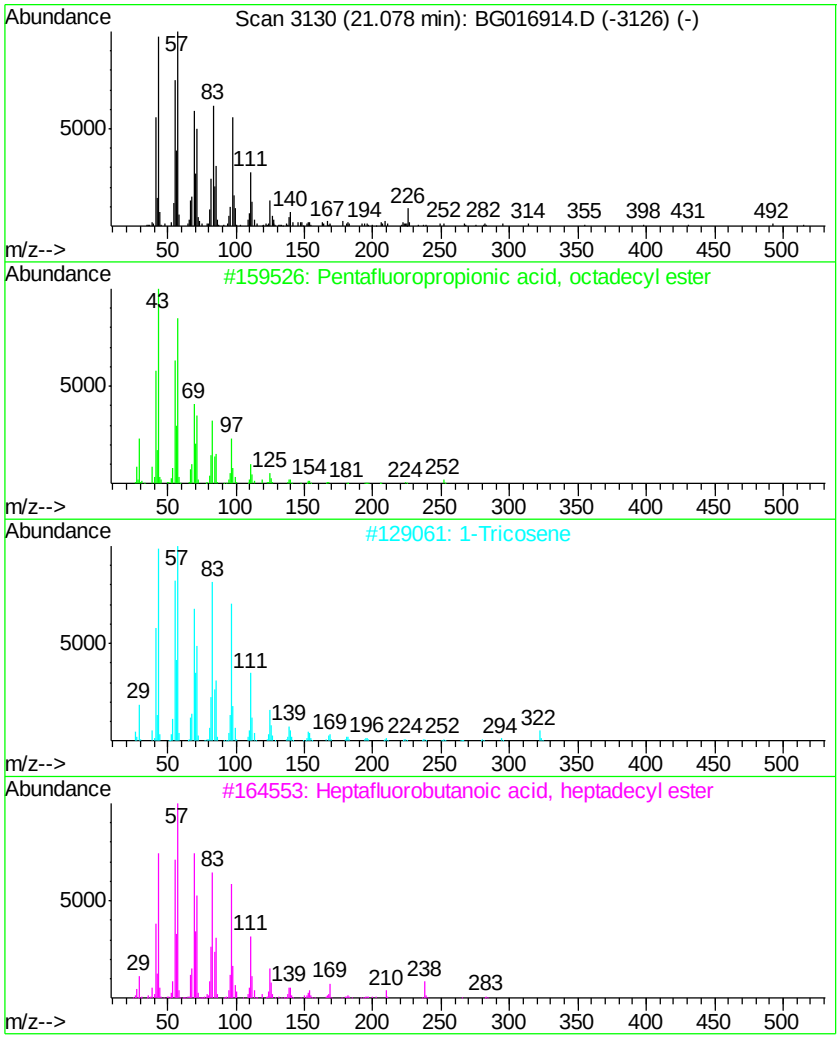
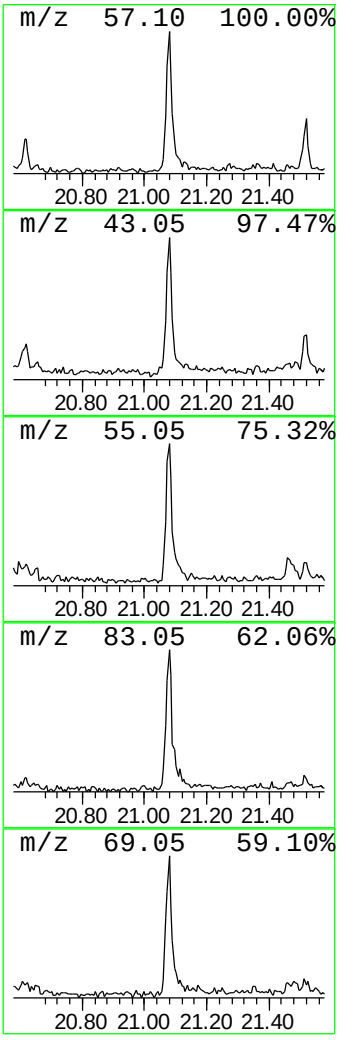
Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	3.78 ng	253936	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4	Cyclooctacosane	392	C28H56	000297-24-5	91
5	Cyclotetracosane	336	C24H48	000297-03-0	91





Tentatively Identified Compound (LSC) summary

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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
unknown2.78	2.78	324.9	ng	7403040	1	7.79	455705	20.0
Butane, 2-methoxy...	3.00	8.7	ng	197388	1	7.79	455705	20.0
2-Pentanone, 4-hy...	4.92	11.2	ng	254465	1	7.79	455705	20.0
unknown7.33	7.33	94.4	ng	2151250	1	7.79	455705	20.0
n-Hexadecanoic acid	18.08	4.2	ng	242932	4	17.18	1165620	20.0
9-Octadecenamide,...	20.50	4.1	ng	276657	5	21.36	1343490	20.0
Pentafluoropropio...	21.08	3.8	ng	253936	5	21.36	1343490	20.0