LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

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-BG071715.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	4.740	344	349	357	rVB	147424	205734	5.97%	0.633%
2	5.198	420	427	435	rBV	1458190	2221952	64.46%	6.832%
3	6.779	687	696	709	rBV	1480105	2387233	69.25%	7.340%
4	7.125	747	755	763	rBV	1684004	2669836	77.45%	8.209%
5	7.590	827	834	842	rBV	407374	633719	18.38%	1.948%
6	7.907	879	888	897	rBV	1228843	1922363	55.77%	5.910%
7	8.741	1023	1030	1041	rVB	929989	1544626	44.81%	4.749%
8	8.894	1050	1056	1066	rBV8	13695	38786	1.13%	0.119%
9	10.369	1299	1307	1313	rBV	563154	918275	26.64%	2.823%
10	12.860	1723	1731	1739	rBV	1918808	2819809	81.80%	8.670%
11	13.706	1869	1875	1884	rVB	600105	844052	24.49%	2.595%
12	14.158	1948	1952	1957	rVB	27055	34783	1.01%	0.107%
13	14.246	1957	1967	1974	rBV2	743160	1171320	33.98%	3.601%
14	14.311	1974	1978	1982	rVB2	26746	35175	1.02%	0.108%
15	14.828	2054	2066	2068	rBV3	59968	190880	5.54%	0.587%
16	15.116	2110	2115	2120	rVB	51955	70032	2.03%	0.215%
17	15.298	2141	2146	2155	rVB2	32024	52359	1.52%	0.161%
18	15.521	2179	2184	2190	rBV6	18551	35277	1.02%	0.108%
19	15.745	2215	2222	2230	rBV	1638077	2442618	70.86%	7.510%
20	15.980	2258	2262	2273	rVB3	57035	109231	3.17%	0.336%
21	16.773	2393	2397	2401	rVV2	47625	57067	1.66%	0.175%
22	16.820	2401	2405	2410	rVB5	23253	34652	1.01%	0.107%
23	16.996	2429	2435	2439	rBV2	843886	1227396	35.61%	3.774%
24	17.037	2439	2442	2448	rVB	263295	352974	10.24%	1.085%
25	17.125	2454	2457	2463	rVB	59683	86271	2.50%	0.265%
26	17.402	2495	2504	2508	rBV4	43449	93705	2.72%	0.288%
27	17.513	2519	2523	2529	rVB4	41273	59435	1.72%	0.183%
28	17.913	2587	2591	2598	rVV2	156773	232616	6.75%	0.715%
29	18.071	2614	2618	2621	rBV2	47923	72357	2.10%	0.222%
30	18.342	2662	2664	2667	rBV4	36974	45614	1.32%	0.140%
31	19.076	2784	2789	2794	rVB	451268	581016	16.86%	1.786%
32	19.129	2795	2798	2803	rVV6	42340	57040	1.65%	0.175%
33	19.205	2808	2811	2817	rVV7	51478	83955	2.44%	0.258%
34	19.435	2841	2850	2859	rBV	364693	631674	18.32%	1.942%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

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-BG071715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.605	2876	2879	2881	rBV2	86042	106092	3.08%	0.326%
36	19.646	2881	2886	2896	rVB	2829734	3447095	100.00%	10.598%
37	19.934	2932	2935	2939	rVB	70512	81803	2.37%	0.252%
38	20.034	2949	2952	2955	rVB	48349	52710	1.53%	0.162%
39	20.639	3051	3055	3059	rBV	252836	271771	7.88%	0.836%
40	20.927	3100	3104	3108	rBV3	170928	227102	6.59%	0.698%
41	21.056	3123	3126	3129	rBV	97209	108293	3.14%	0.333%
42	21.197	3141	3150	3154	rBV2	1160017	1876333	54.43%	5.769%
43	21.232	3154	3156	3162	rVB	208359	268114	7.78%	0.824%
44	21.538	3205	3208	3215	rVB	215911	274600	7.97%	0.844%
45	22.754	3411	3415	3420	rBV	156711	306008	8.88%	0.941%
46	23.318	3507	3511	3520	rVB	163180	315441	9.15%	0.970%
47	23.418	3522	3528	3534	rBV	632751	1225448	35.55%	3.768%

Sum of corrected areas: 32524642

Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
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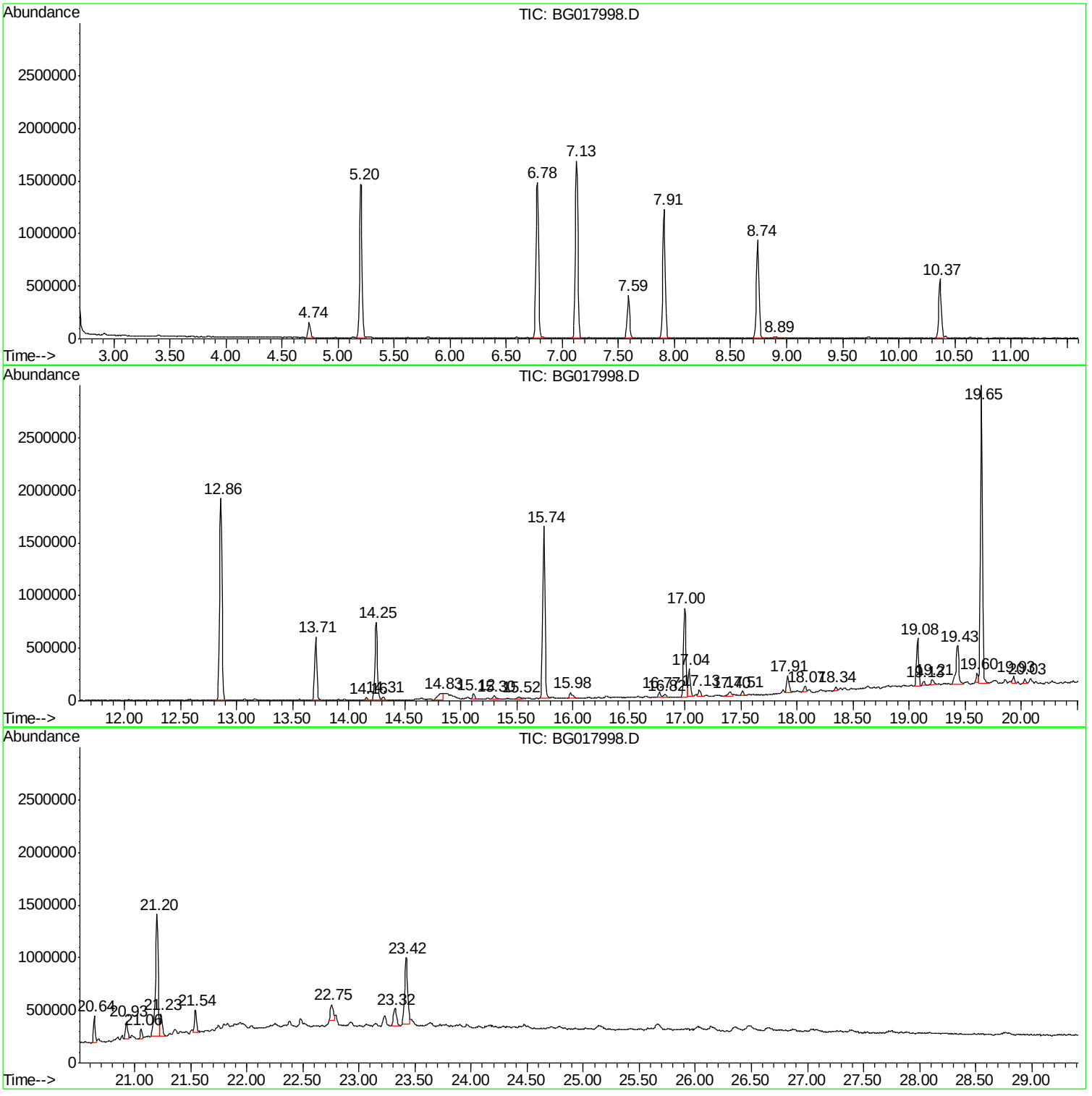
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

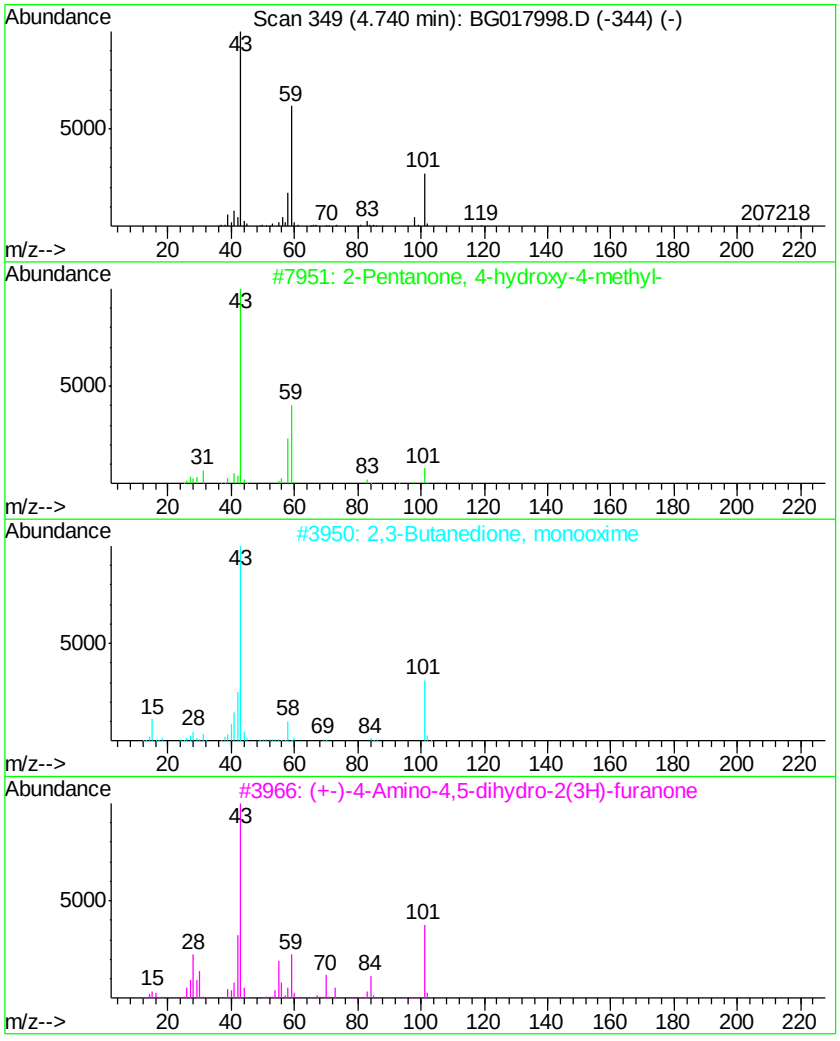
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

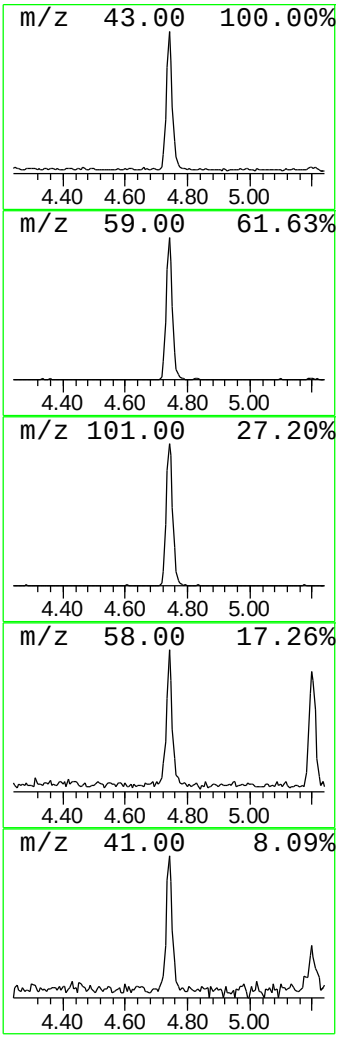
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	6.49 ng	205734	1,4-Dichlorobenzene-d4	7.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17
4	3-Hexanol	102	C6H14O	000623-37-0	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

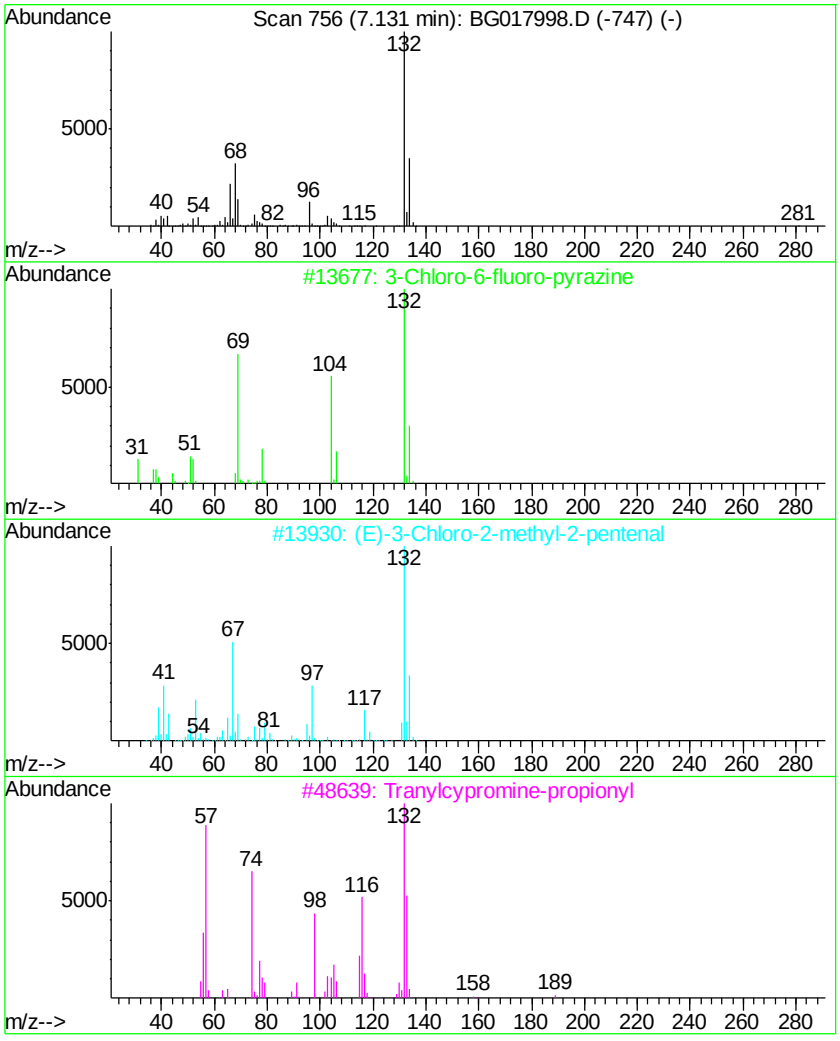
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

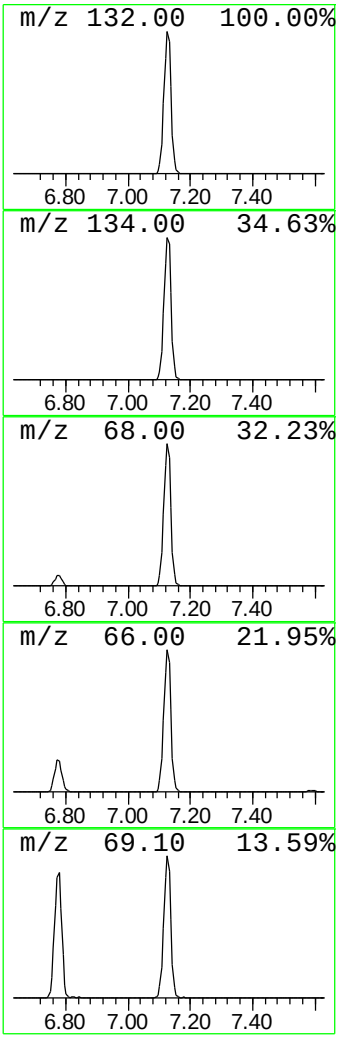
****

Peak Number 2 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	84.26 ng	2669840	1,4-Dichlorobenzene-d4	7.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

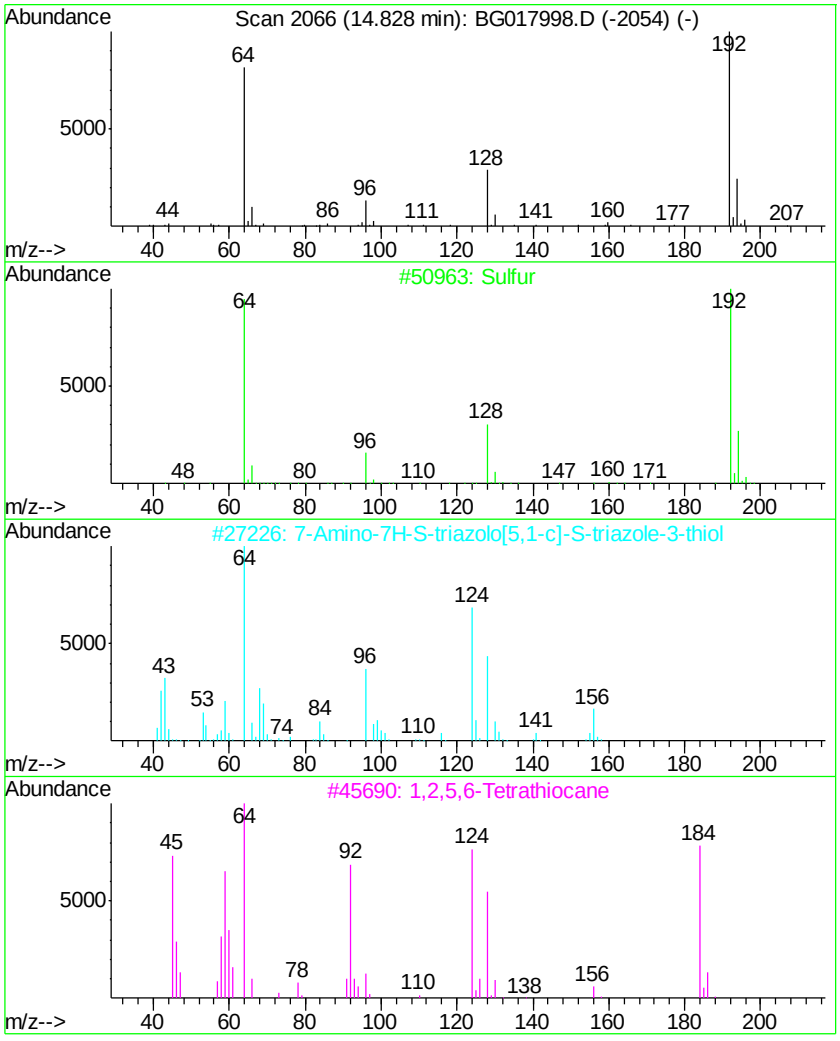
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

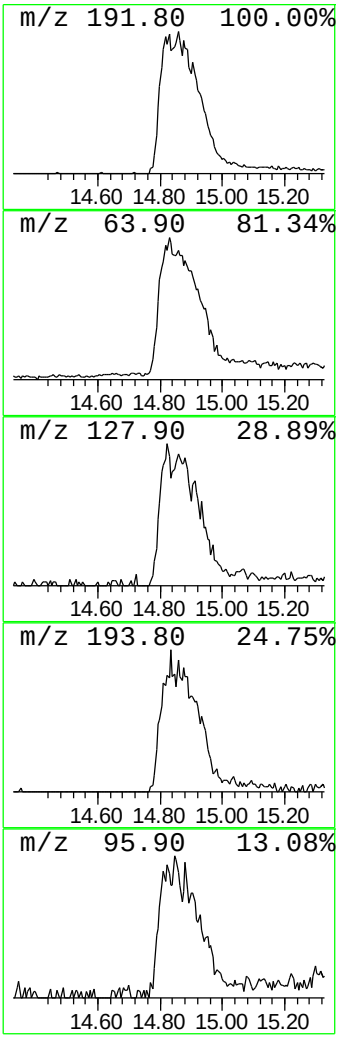
****

Peak Number 4 Sulfur Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.26 ng	190880	Acenaphthene-d10	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur	192	S6	013798-23-7	97
2	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	38
3	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	36
4	Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	9
5	Pyridine-3,5-dicarbonitrile, 2-a...	192	C8H5ClN4	064829-09-0	9





Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

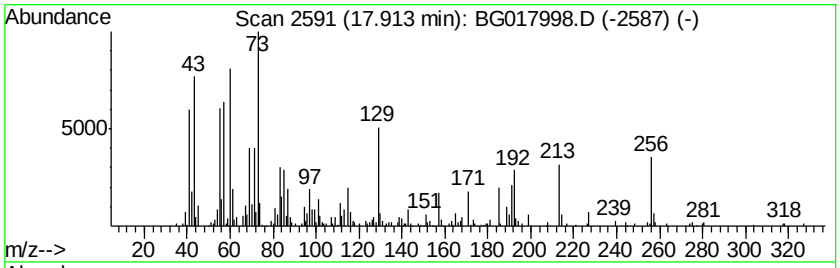
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

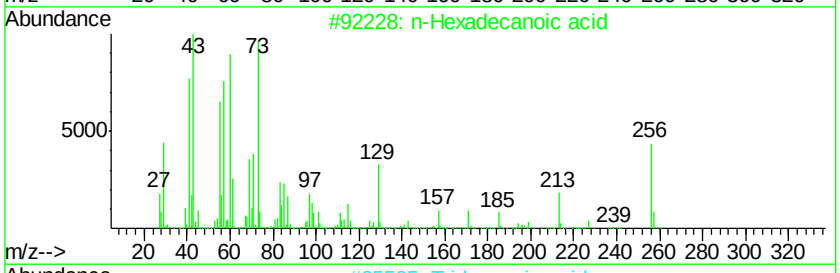
****

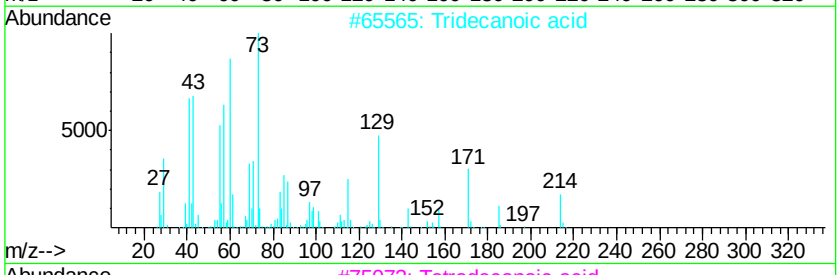
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

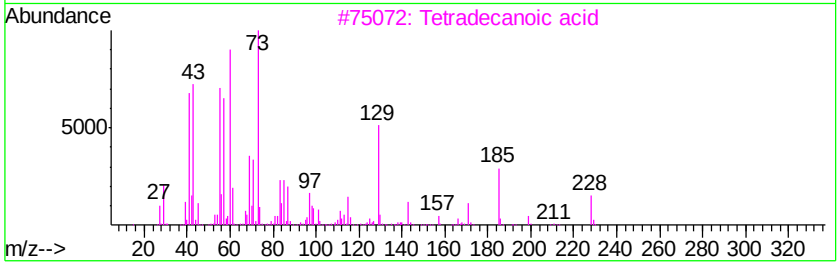
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	3.79 ng	232616	Phenanthrene-d10	17.00

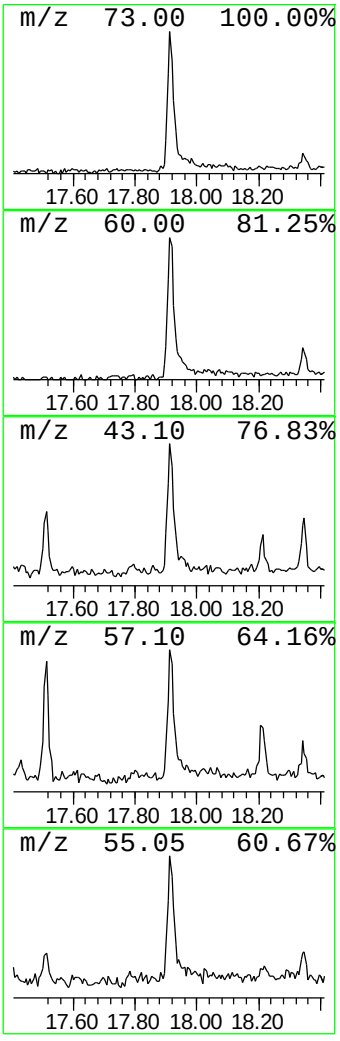
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	35











Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

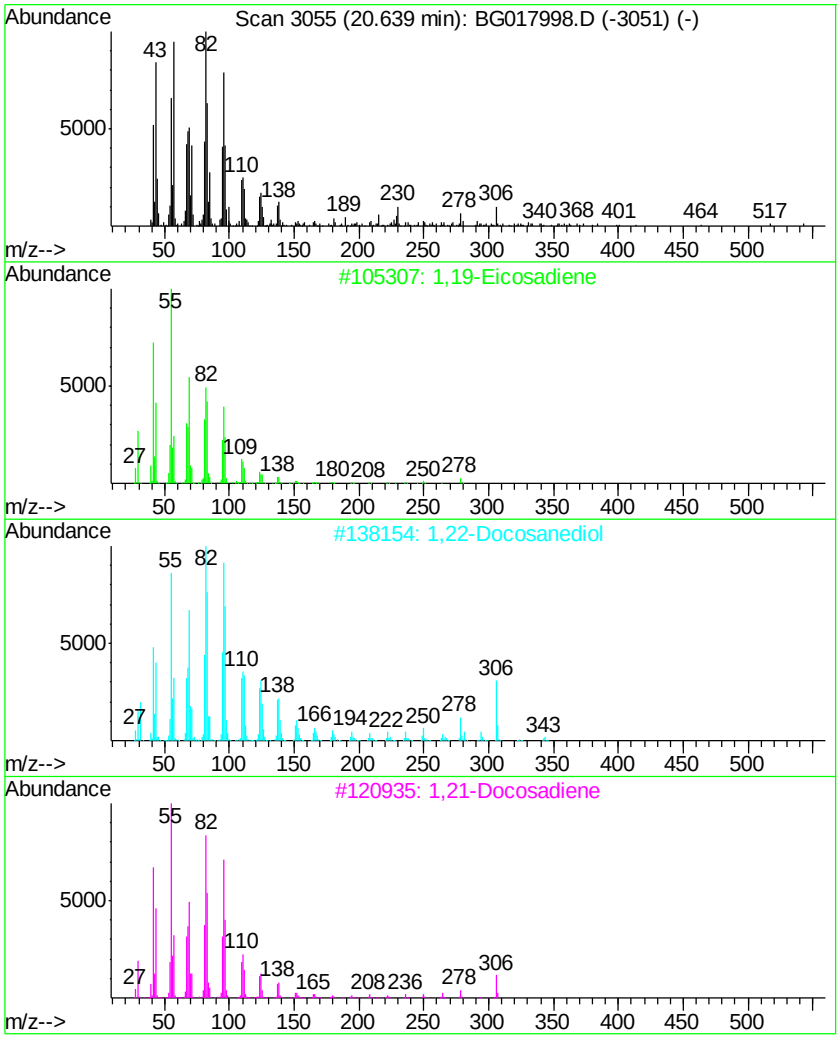
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

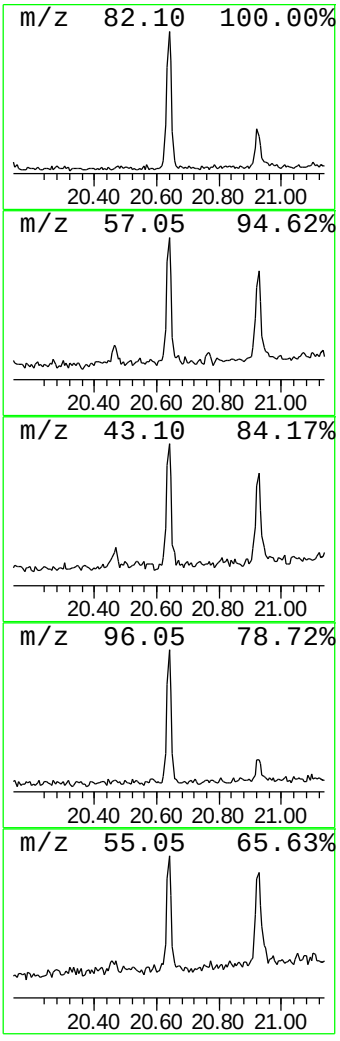
****

Peak Number 6 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.64	2.90 ng	271771	Chrysene-d12	21.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	96
2	1,22-Docosanediol	342	C22H46O2	022513-81-1	95
3	1,21-Docosadiene	306	C22H42	053057-53-7	95
4	Bicyclo[10.8.0]eicosane, (E)-	278	C20H38	1000155-85-0	93
5	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	92





Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

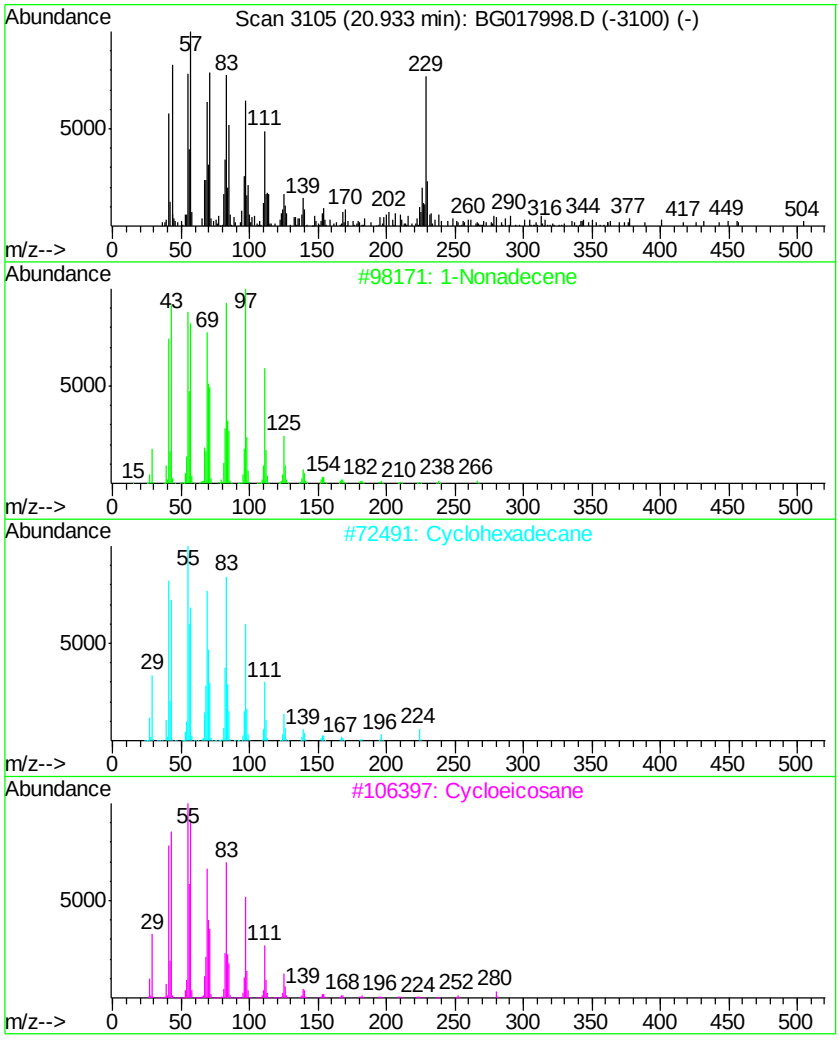
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

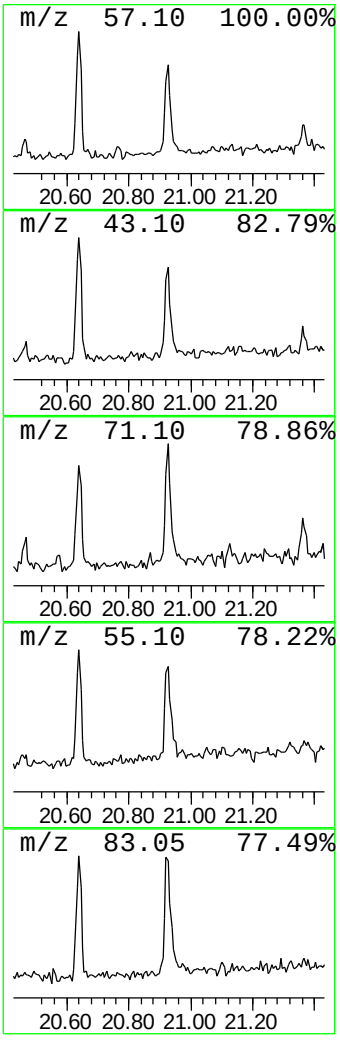
****

Peak Number 7 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	2.42 ng	227102	Chrysene-d12	21.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	Cyclohexadecane	224	C16H32	000295-65-8	87
3	Cycloeicosane	280	C20H40	000296-56-0	78
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	74
5	Cyclopentadecane	210	C15H30	000295-48-7	64





Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

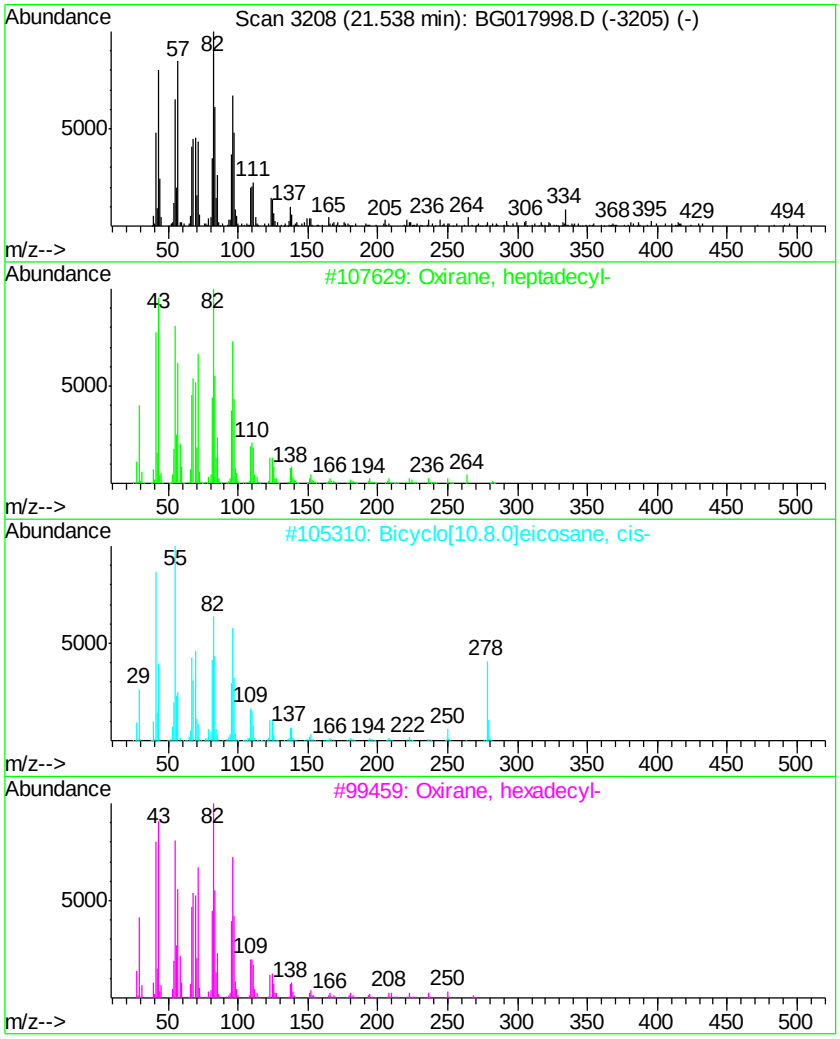
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

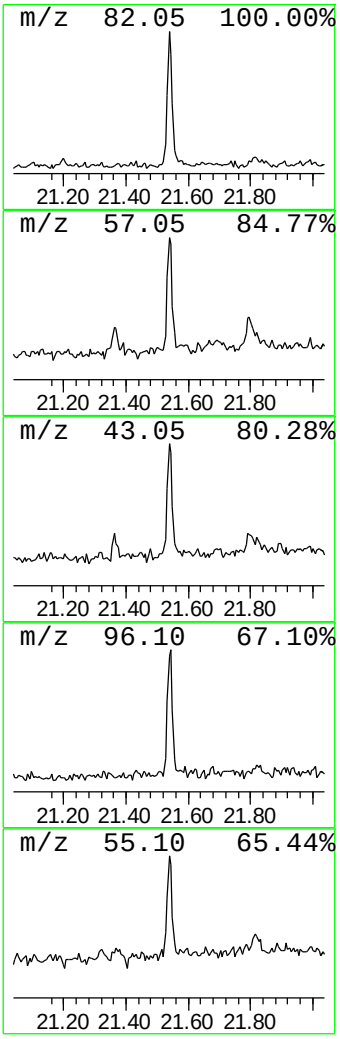
****

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.54	2.93 ng	274600	Chrysene-d12	21.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Octadecanal	268	C18H36O	000638-66-4	91
5	16-Octadecenal	266	C18H34O	056554-87-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\Data\BG072015\
Data File : BG017998.D
Acq On : 20 Jul 2015 20:37
Operator : TP/UM
Sample : G3024-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : UST-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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
2-Pentanone, 4-hy...	4.74	6.5	ng	205734	1	7.59	633719	20.0
unknown7.13	7.13	84.3	ng	2669840	1	7.59	633719	20.0
Sulfur	14.83	3.3	ng	190880	3	14.25	1171320	20.0
n-Hexadecanoic acid	17.91	3.8	ng	232616	4	17.00	1227400	20.0
1,19-Eicosadiene	20.64	2.9	ng	271771	5	21.20	1876330	20.0
1-Nonadecene	20.93	2.4	ng	227102	5	21.20	1876330	20.0
Oxirane, heptadecyl-	21.54	2.9	ng	274600	5	21.20	1876330	20.0