LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016250.D
Acq On : 7 Apr 2015 11:22
Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

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-BG040615.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	2.799	14	19	29	rBV	990907	1490634	37.29%	5.777%
2	2.875	29	32	37	rVV	128343	149693	3.74%	0.580%
3	4.808	355	361	369	rBV	157546	220136	5.51%	0.853%
4	5.278	435	441	449	rBV	1202128	1684632	42.14%	6.529%
5	6.870	704	712	725	rBV	1258162	1975584	49.42%	7.656%
6	7.229	766	773	783	rBV	1181621	1881434	47.06%	7.292%
7	7.699	845	853	860	rBV	235809	364144	9.11%	1.411%
8	8.016	900	907	914	rBV	857762	1339198	33.50%	5.190%
9	8.856	1042	1050	1061	rBV	694481	1137239	28.45%	4.407%
10	10.484	1318	1327	1333	rBV	365489	594816	14.88%	2.305%
11	12.957	1741	1748	1759	rBV	1837113	2656956	66.46%	10.297%
12	13.791	1885	1890	1899	rVB	102278	139845	3.50%	0.542%
13	14.338	1976	1983	1990	rBV2	593433	850837	21.28%	3.297%
14	15.695	2209	2214	2221	rVB	79123	107333	2.68%	0.416%
15	15.824	2230	2236	2251	rBV	1315454	1826161	45.68%	7.077%
16	17.076	2443	2449	2455	rBV2	786119	1090306	27.27%	4.226%
17	17.981	2597	2603	2613	rBV	218144	347153	8.68%	1.345%
18	19.138	2793	2800	2808	rBV	26414	45441	1.14%	0.176%
19	19.262	2816	2821	2830	rBV2	91990	151858	3.80%	0.589%
20	19.708	2891	2897	2907	rBV	3166781	3997789	100.00%	15.494%
21	20.971	3107	3112	3123	rBV	476608	675051	16.89%	2.616%
22	21.171	3142	3146	3155	rVB	265969	300650	7.52%	1.165%
23	21.259	3155	3161	3166	rBV	948529	1242595	31.08%	4.816%
24	21.859	3257	3263	3273	rVB6	21902	59414	1.49%	0.230%
25	22.434	3356	3361	3367	rVB2	53737	82932	2.07%	0.321%
26	22.810	3421	3425	3431	rBV3	24090	46470	1.16%	0.180%
27	23.386	3518	3523	3531	rVB5	20070	44983	1.13%	0.174%
28	23.504	3535	3543	3559	rBV2	628429	1172666	29.33%	4.545%
29	24.038	3630	3634	3641	rVB4	21087	40691	1.02%	0.158%
30	24.126	3643	3649	3656	rBV5	36921	86232	2.16%	0.334%

Sum of corrected areas: 25802873

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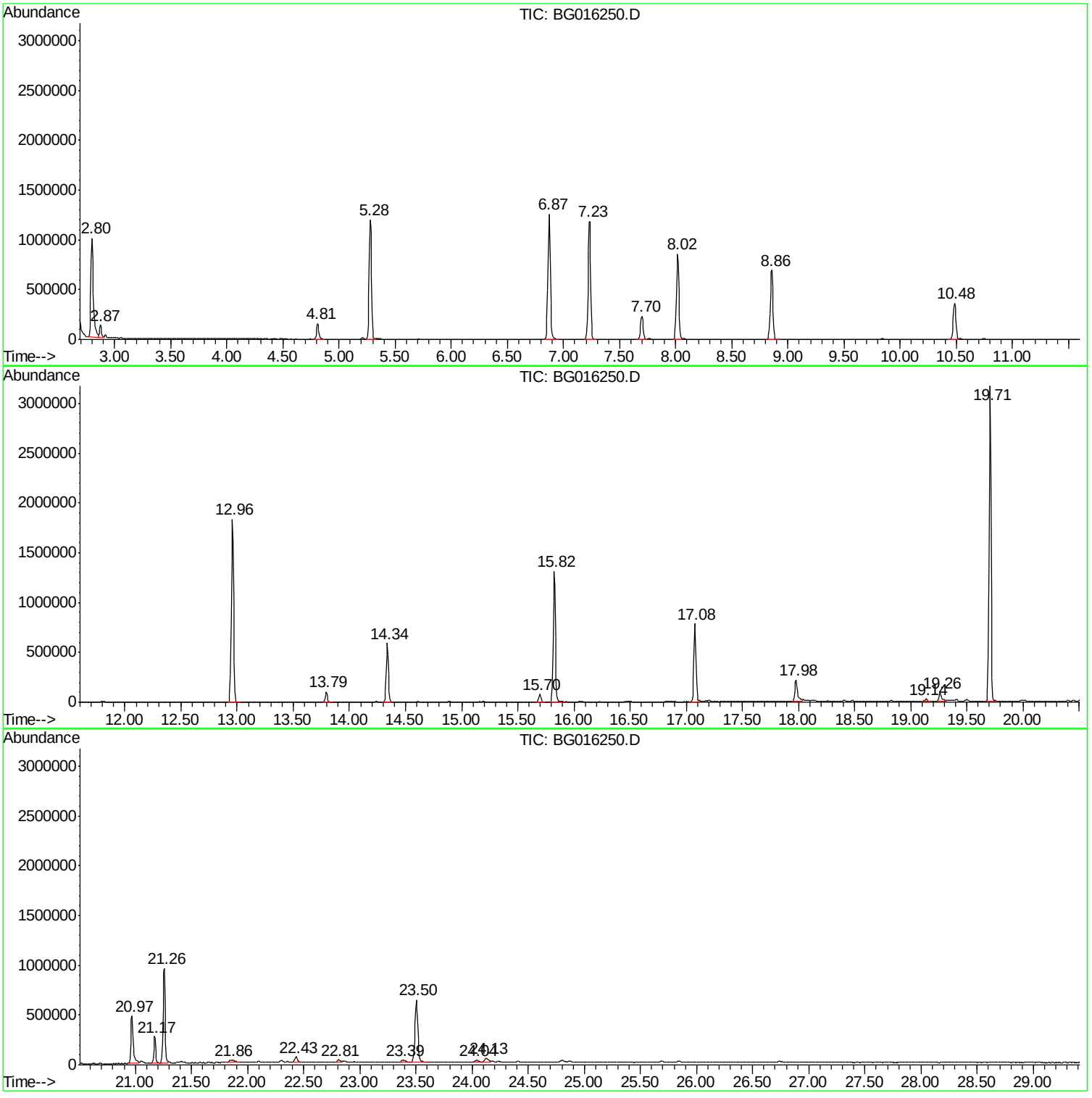
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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Data File : BG016250.D
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Sample : G1779-10
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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

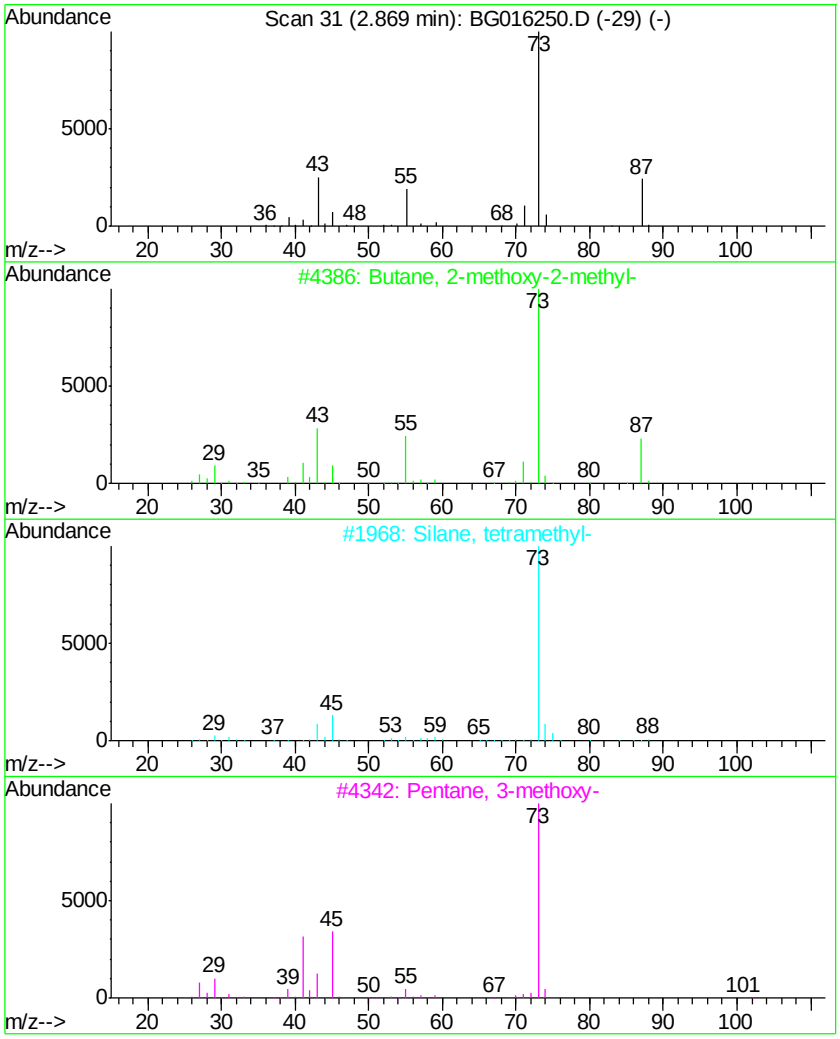
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

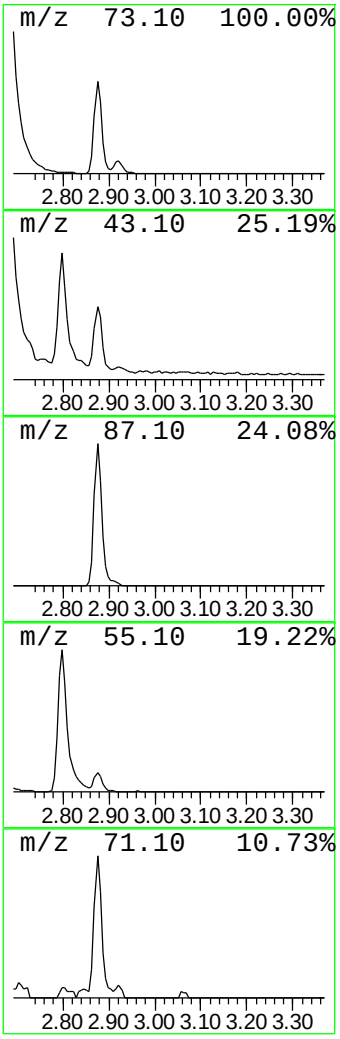
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	8.22 ng	149693	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	7
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





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Data File : BG016250.D
Acq On : 7 Apr 2015 11:22
Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

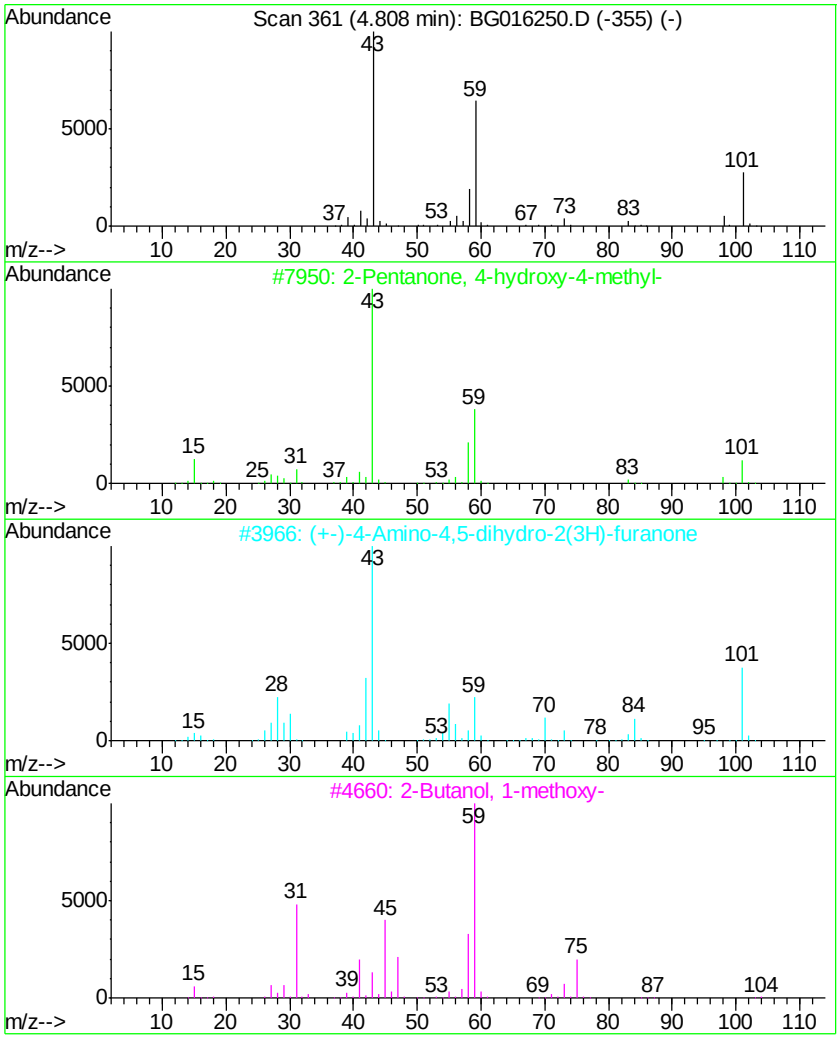
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

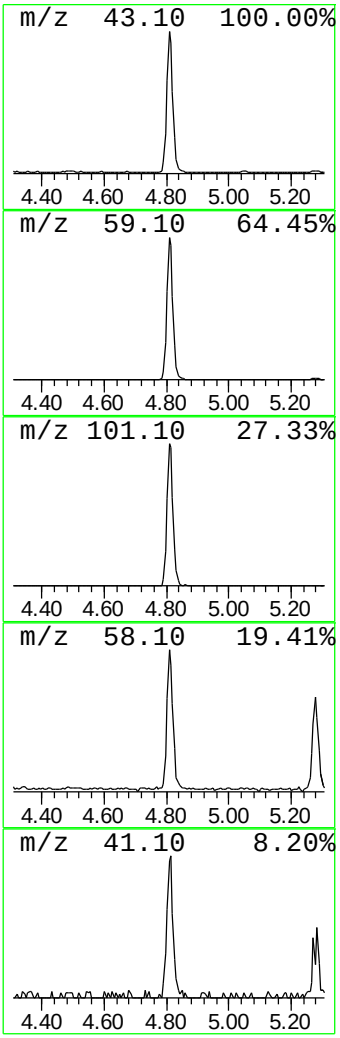
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	12.09 ng	220136	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016250.D
Acq On : 7 Apr 2015 11:22
Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

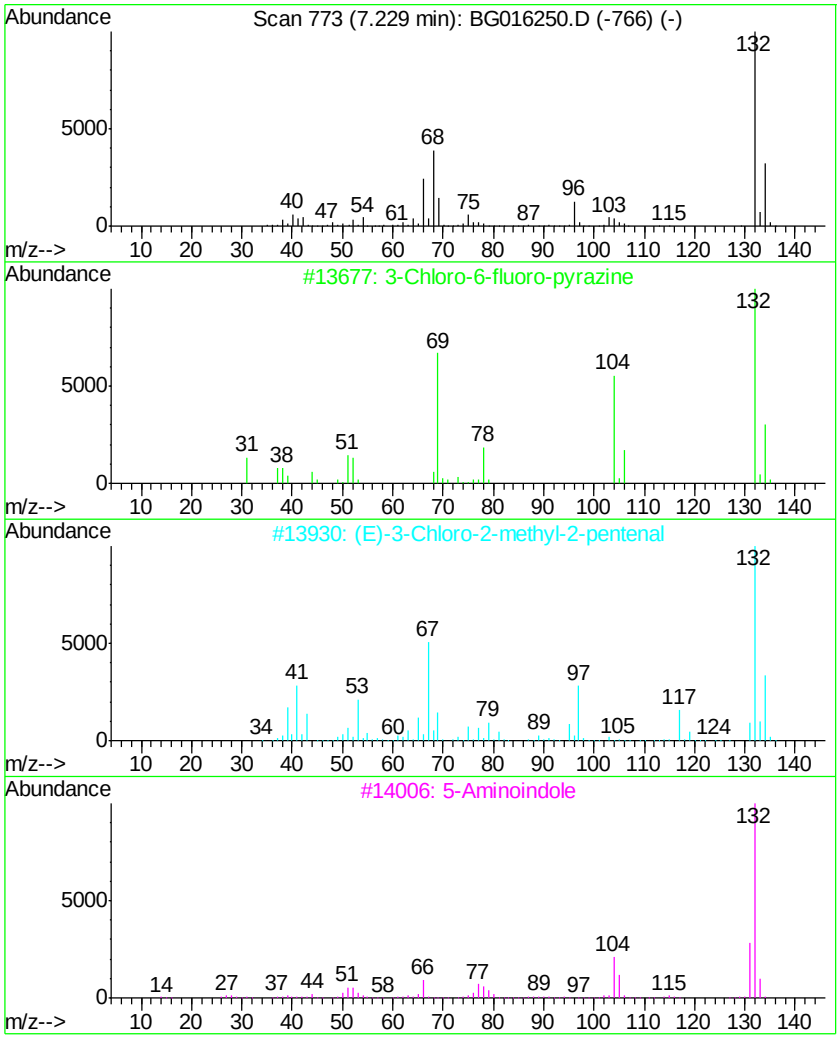
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

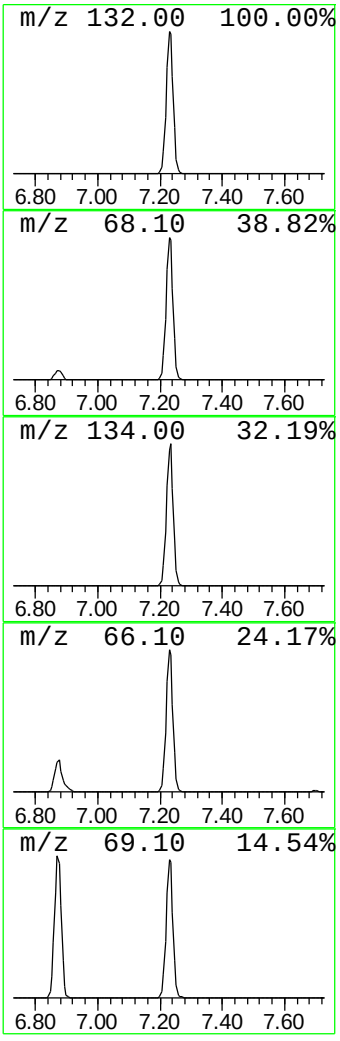
****

Peak Number 4 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	103.34 ng	1881430	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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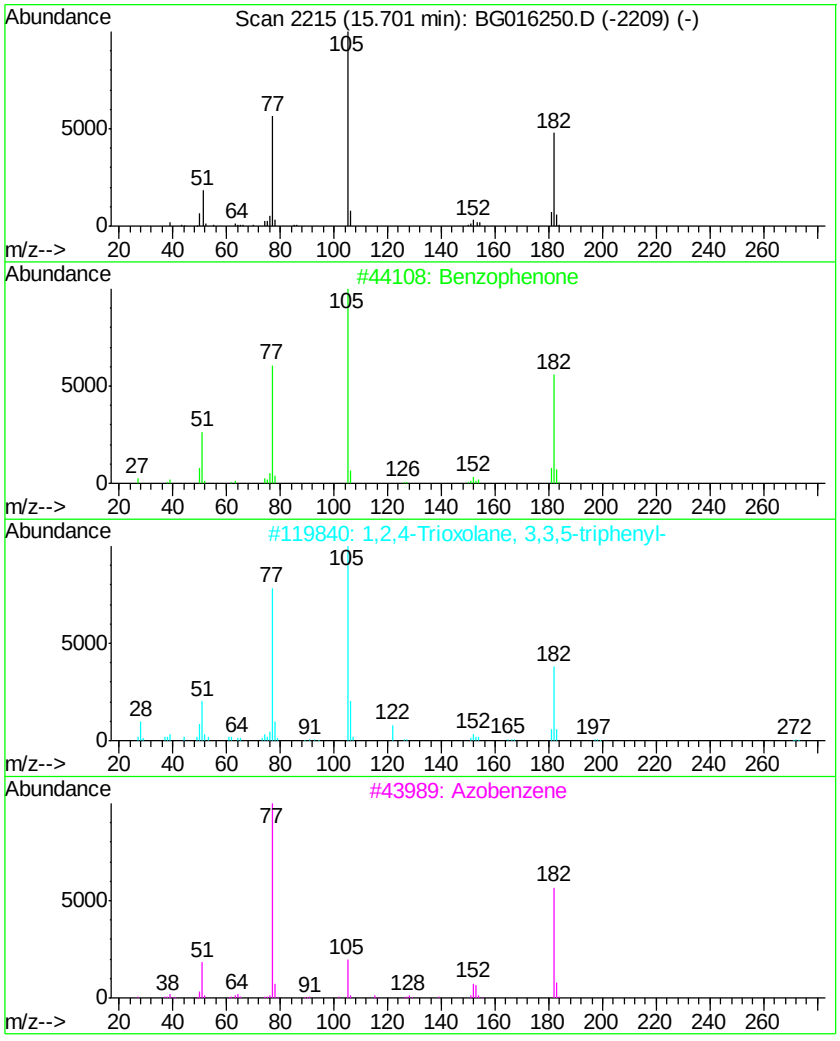
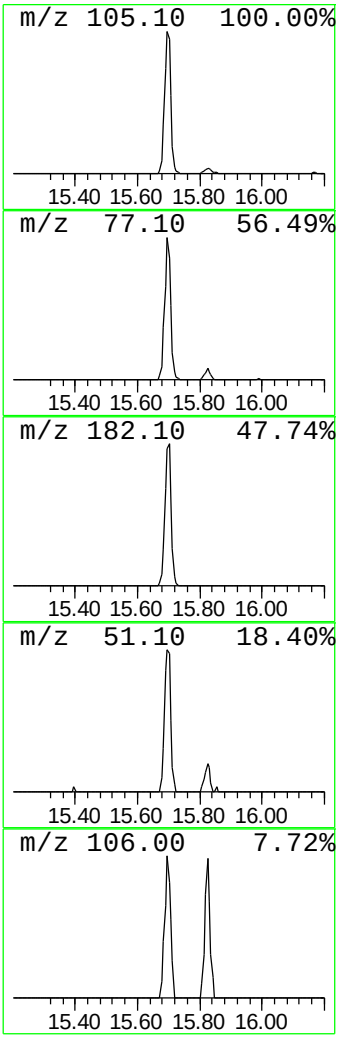
Peak Number 6 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.52 ng	107333	Acenaphthene-d10	14.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	78
3	Azobenzene	182	C12H10N2	000103-33-3	64
4	.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016250.D
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Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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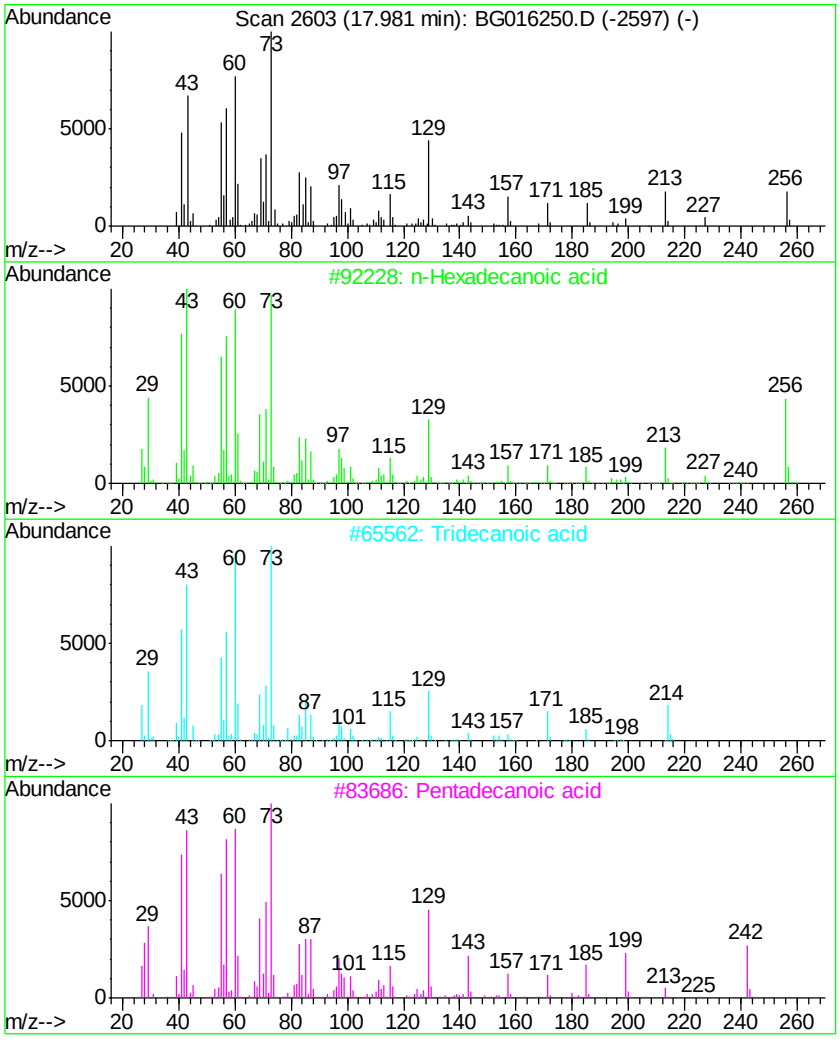
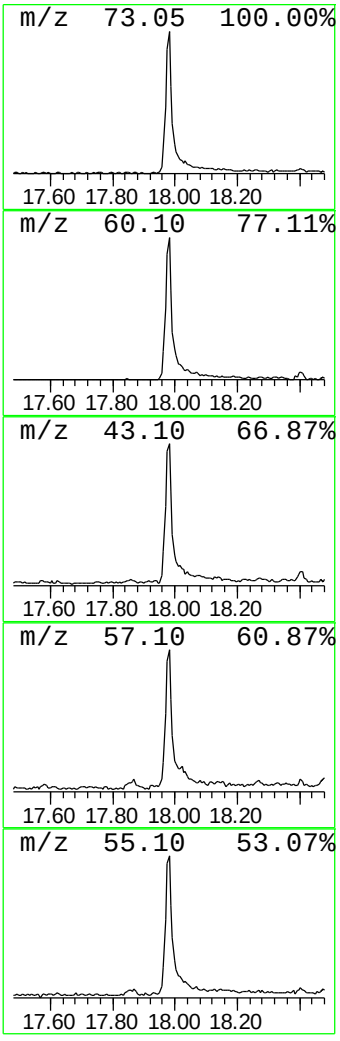
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	6.37 ng	347153	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Operator : TP/IZ
Sample : G1779-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

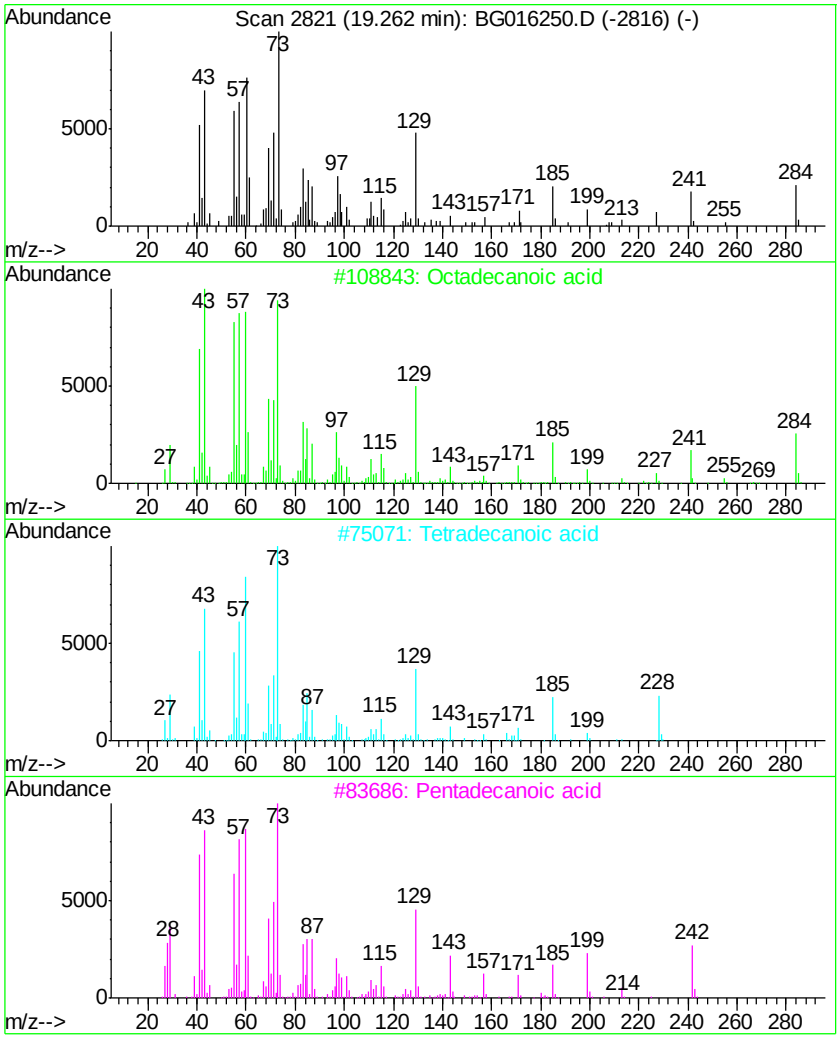
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

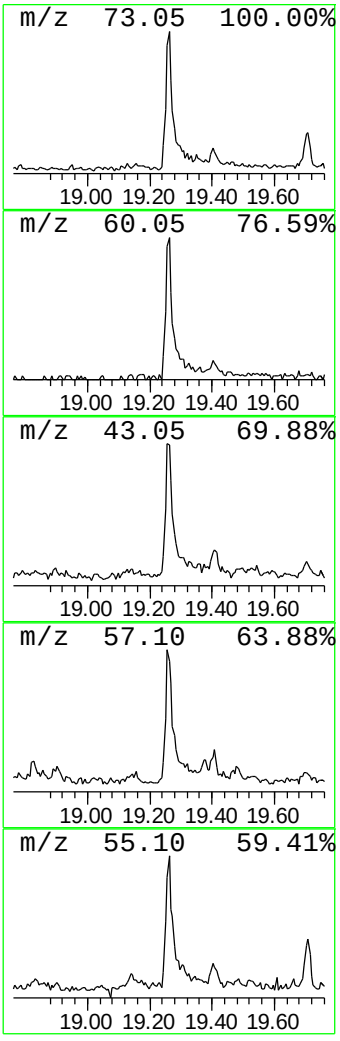
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	2.44 ng	151858	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Tridecane	184	C13H28	000629-50-5	11





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-5(1-3)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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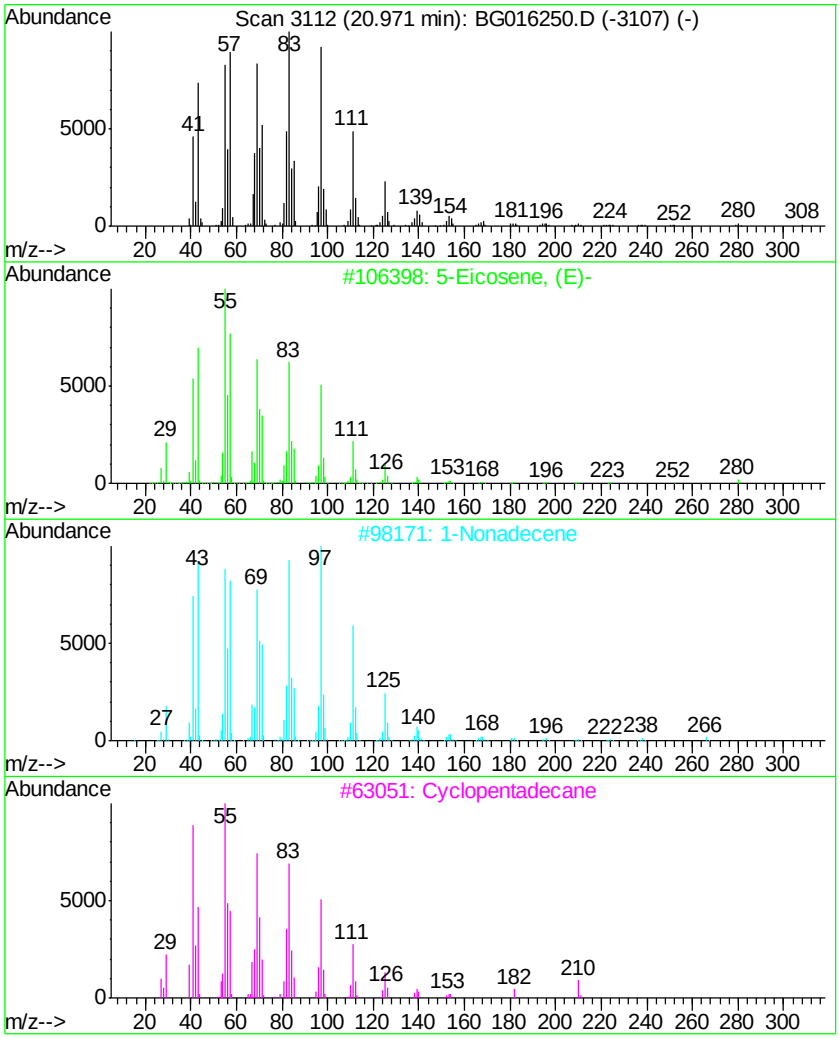
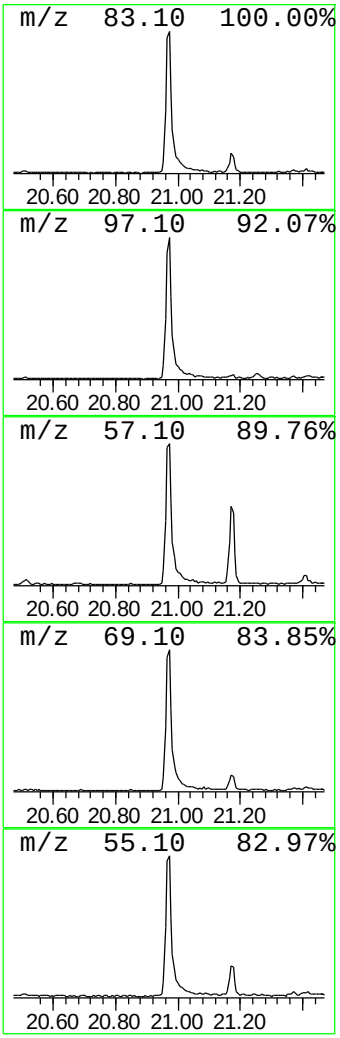
Peak Number 9 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	10.87 ng	675051	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Nonadecene	266	C19H38	018435-45-5	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
5	1-Eicosanol	298	C20H42O	000629-96-9	90





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : SB-5(1-3)

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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
Butane, 2-methoxy...	2.87	8.2	ng	149693	1	7.70	364144	20.0
2-Pentanone, 4-hy...	4.81	12.1	ng	220136	1	7.70	364144	20.0
unknown7.23	7.23	103.3	ng	1881430	1	7.70	364144	20.0
Benzophenone	15.70	2.5	ng	107333	3	14.34	850837	20.0
n-Hexadecanoic acid	17.98	6.4	ng	347153	4	17.08	1090310	20.0
Octadecanoic acid	19.26	2.4	ng	151858	5	21.26	1242600	20.0
5-Eicosene, (E)-	20.97	10.9	ng	675051	5	21.26	1242600	20.0