LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

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_F\METHODS\8270-BF011415.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	1.327	20	21	26	rBV	8953	18718	1.88%	0.266%
2	1.407	26	28	34	rVB	15389	32604	3.28%	0.464%
3	3.830	237	240	251	rBV	70976	179606	18.05%	2.554%
4	4.790	321	324	338	rBB	358604	679843	68.31%	9.668%
5	7.167	529	532	536	rBV	395270	637812	64.09%	9.070%
6	7.247	536	539	548	rVB	438115	724663	72.81%	10.306%
7	7.762	581	584	588	rBV	89639	143941	14.46%	2.047%
8	8.082	609	612	616	rBV	343858	527722	53.03%	7.505%
9	9.065	695	698	705	rBV	272465	419348	42.14%	5.964%
10	10.676	835	839	842	rBV	120089	205525	20.65%	2.923%
11	13.328	1067	1071	1074	rBV	558570	825885	82.99%	11.745%
12	14.803	1196	1200	1203	rBV	123795	222548	22.36%	3.165%
13	16.517	1347	1350	1353	rBV	338470	488267	49.06%	6.944%
14	17.626	1445	1447	1450	rBV	190945	237056	23.82%	3.371%
15	19.317	1593	1595	1598	rVB	22467	27587	2.77%	0.392%
16	19.786	1633	1636	1638	rBB	65112	76563	7.69%	1.089%
17	19.877	1641	1644	1646	rVB	875360	995219	100.00%	14.153%
18	20.677	1712	1714	1716	rBV	46905	51411	5.17%	0.731%
19	20.803	1723	1725	1727	rBB	6823	10092	1.01%	0.144%
20	21.135	1752	1754	1757	rBV	236089	254022	25.52%	3.612%
21	22.780	1895	1898	1901	rBV	195377	232777	23.39%	3.310%
22	23.649	1972	1974	1978	rVB2	7372	11668	1.17%	0.166%
23	24.301	2027	2031	2034	rBV3	15137	28890	2.90%	0.411%

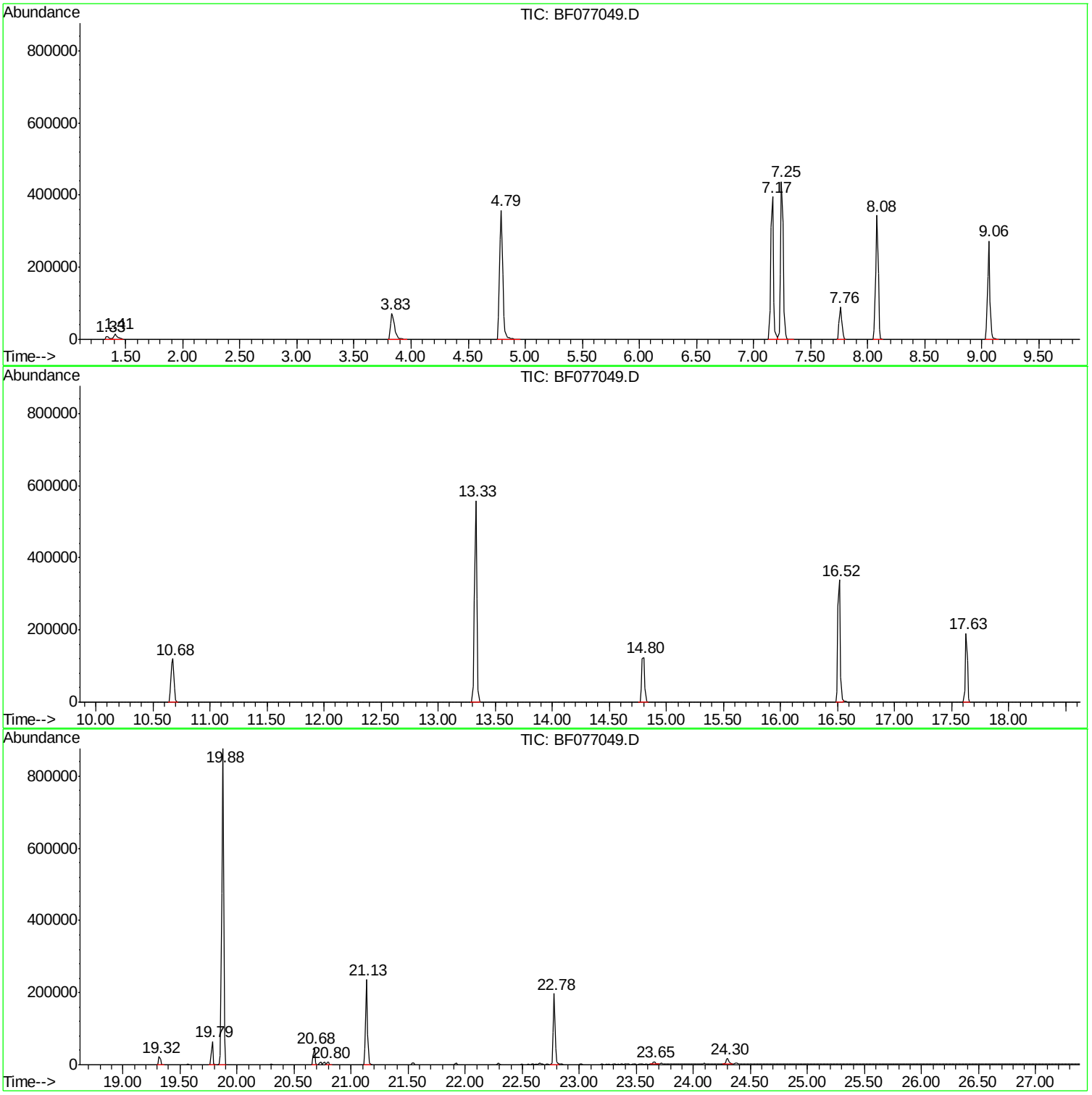
Sum of corrected areas: 7031767

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

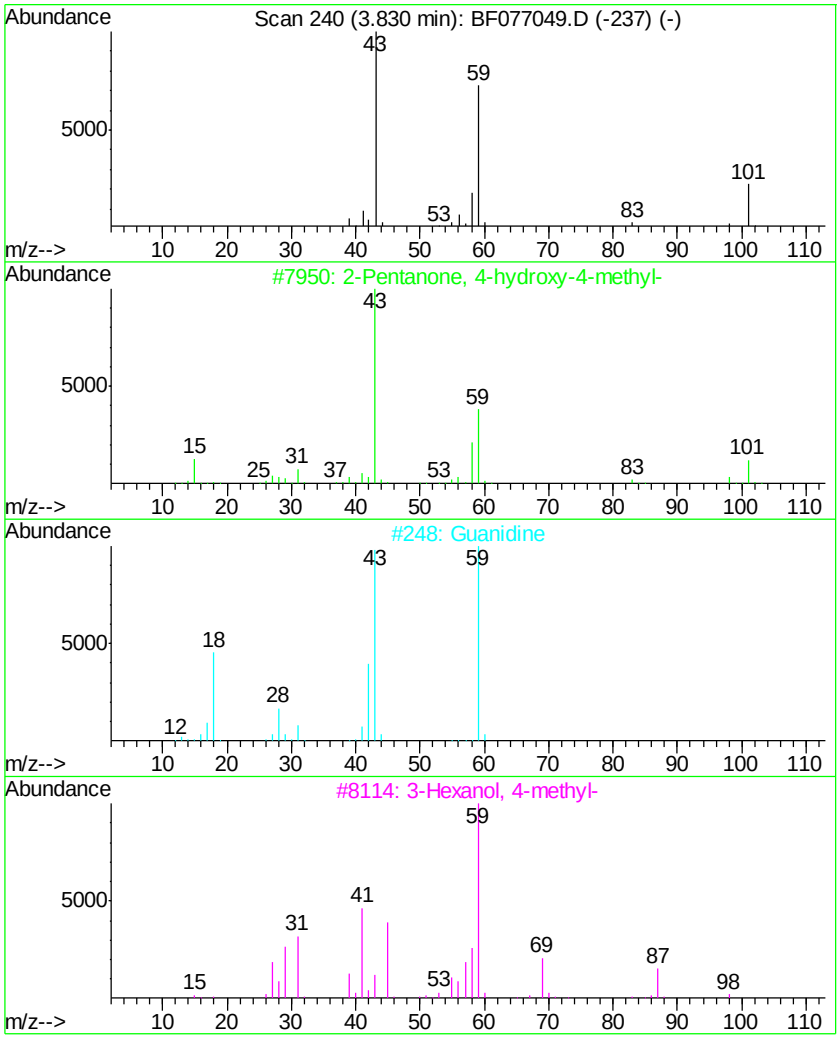
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

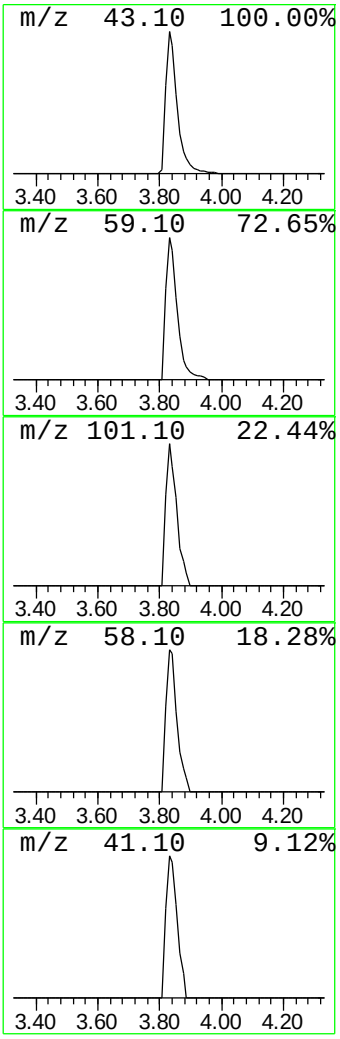
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.83	24.96 ng	179606	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

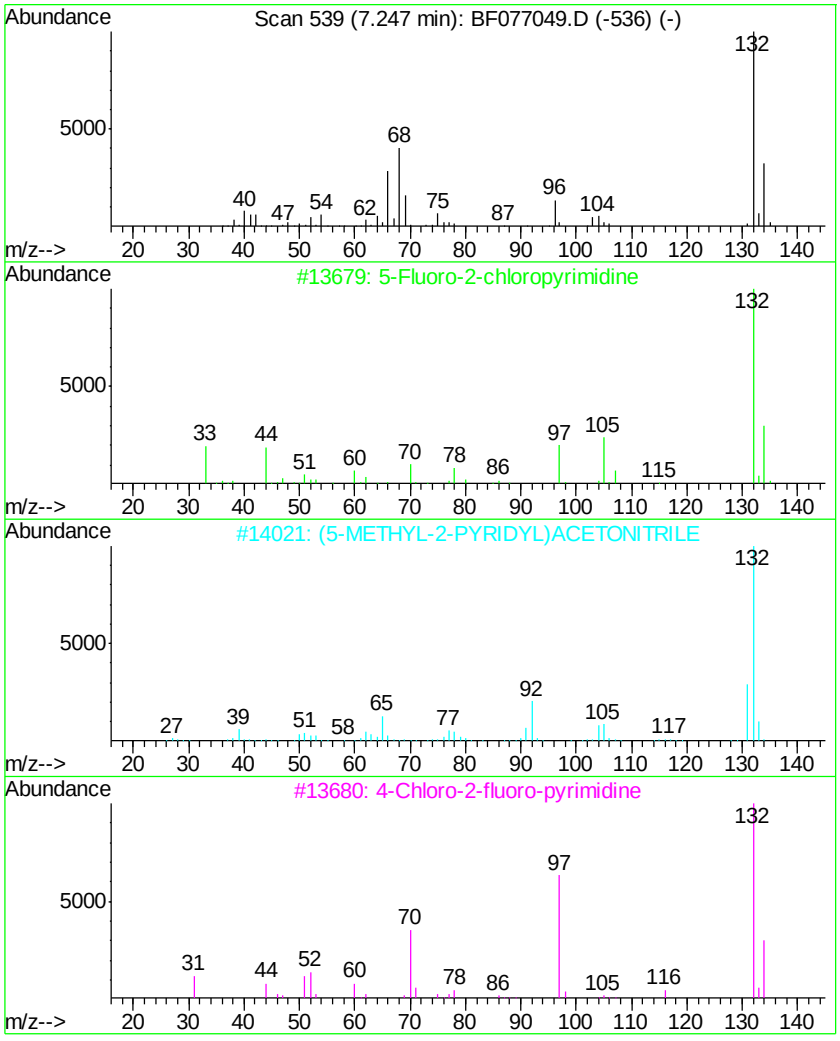
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

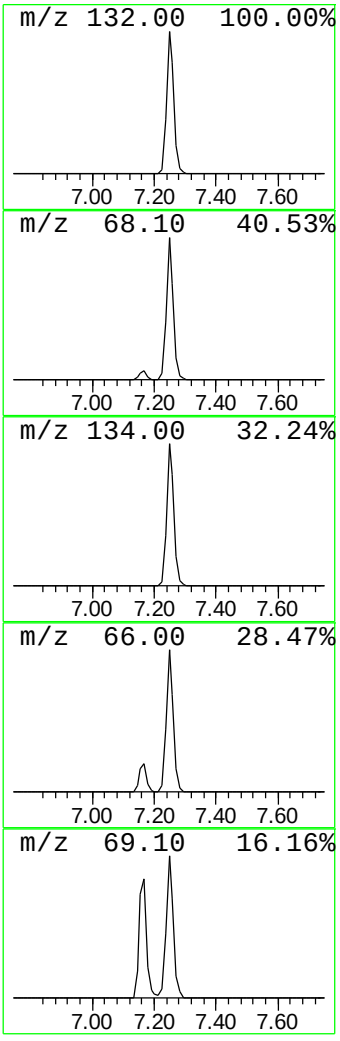
****

Peak Number 4 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	100.69 ng	724663	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

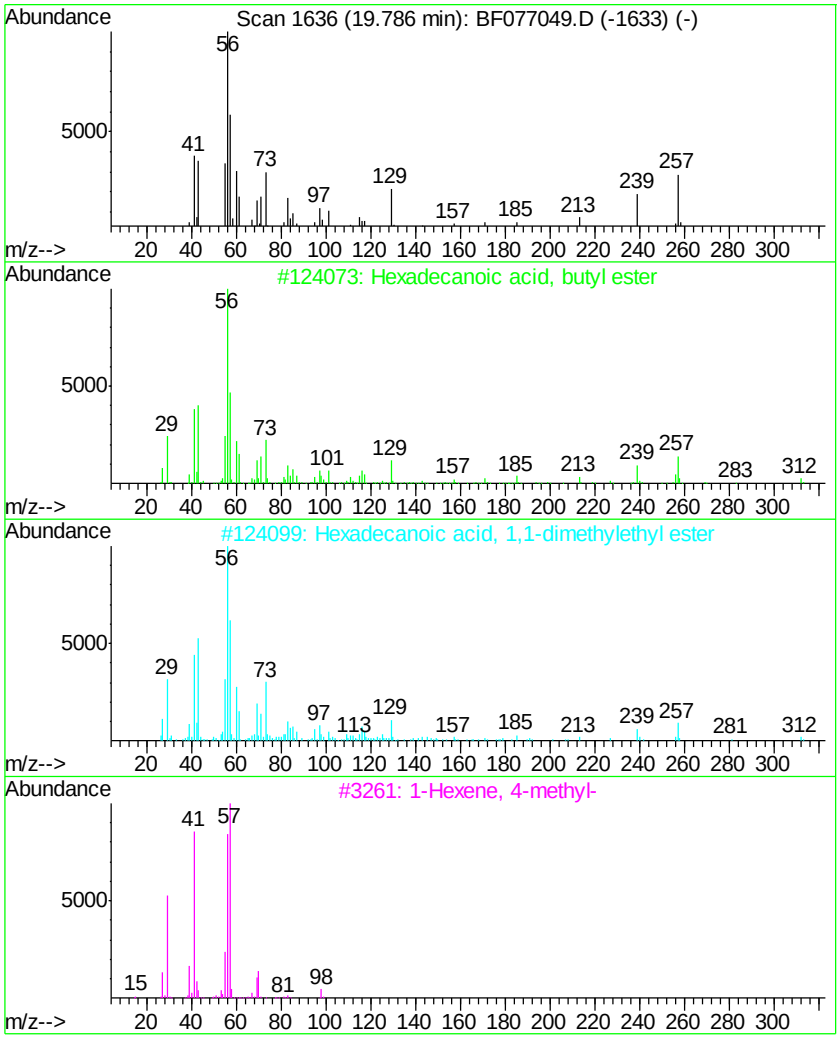
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

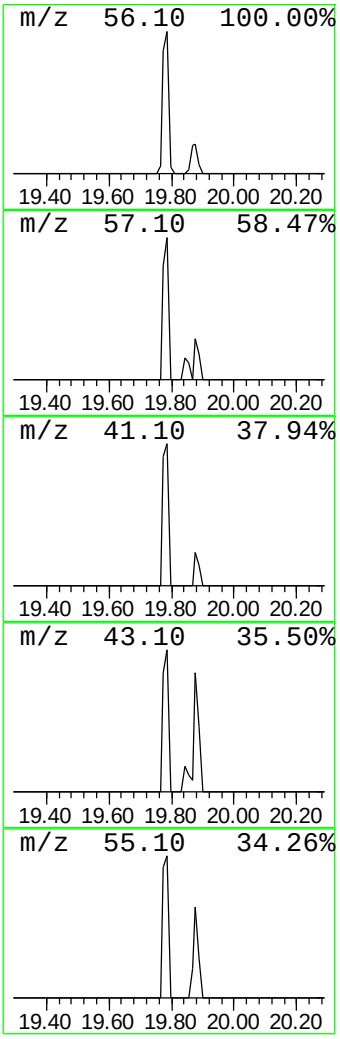
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	6.03 ng	76563	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

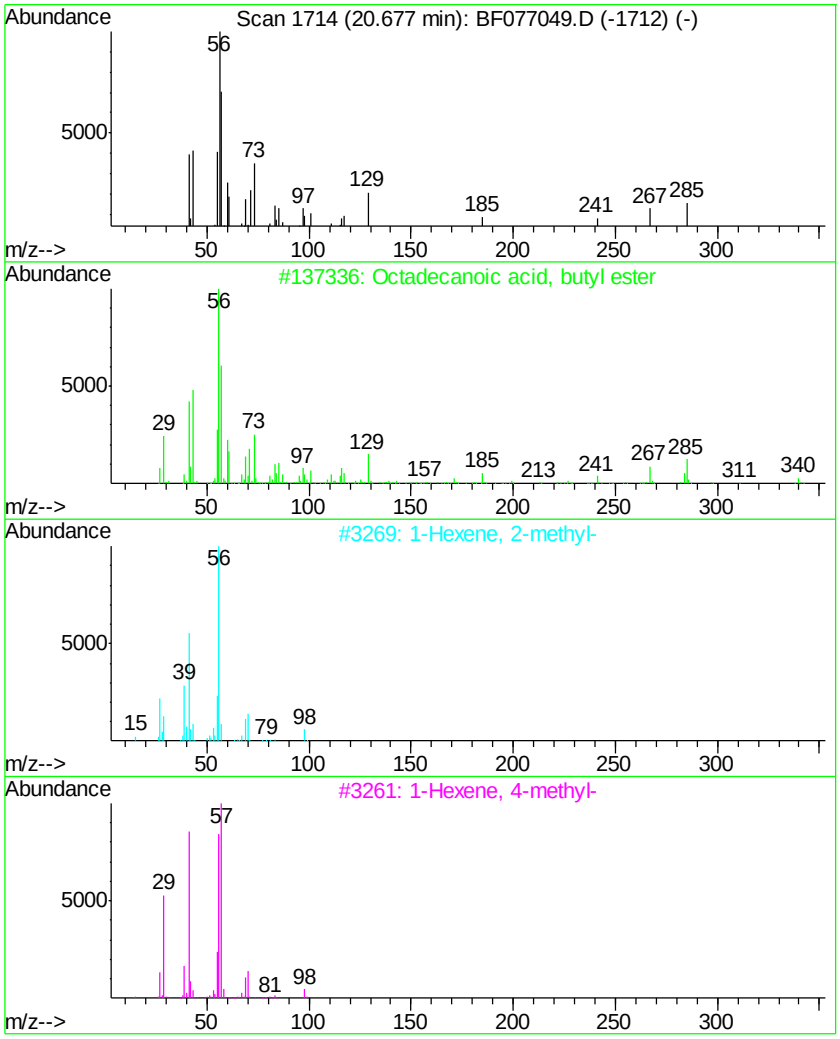
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

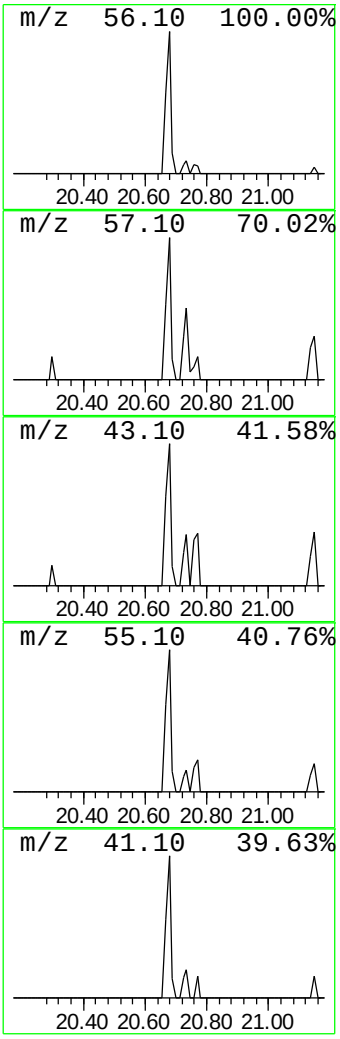
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.68	4.05 ng	51411	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
3	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	35
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

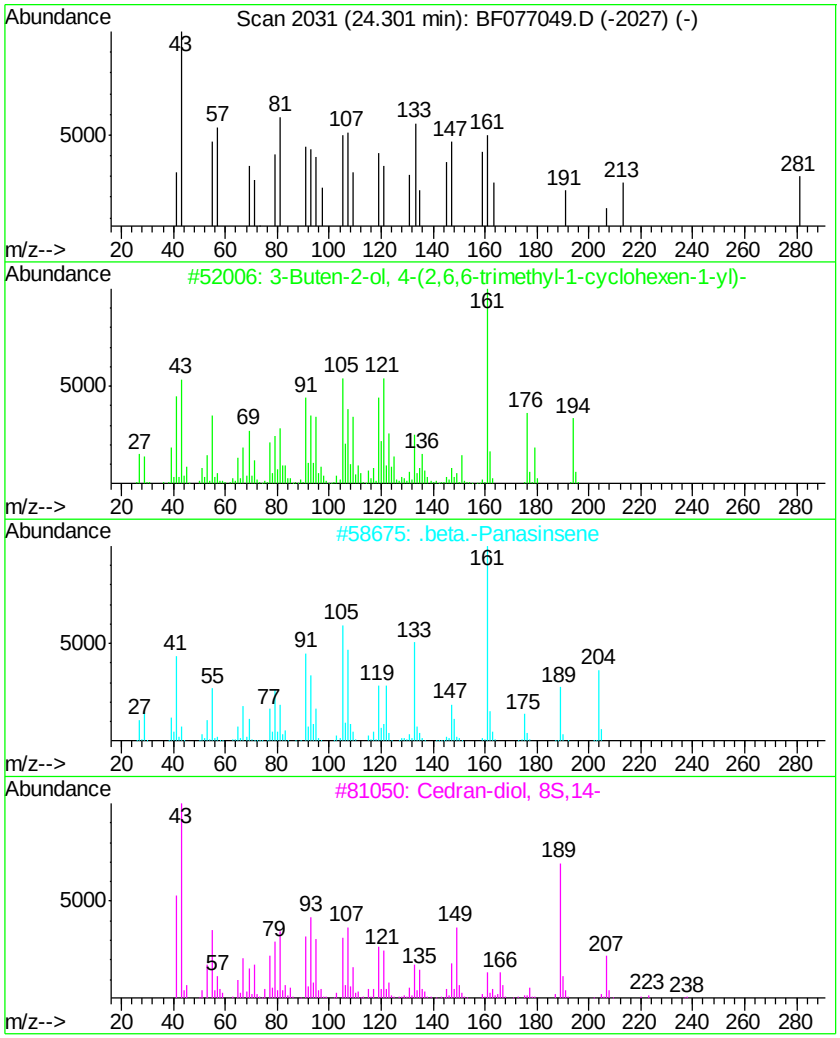
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

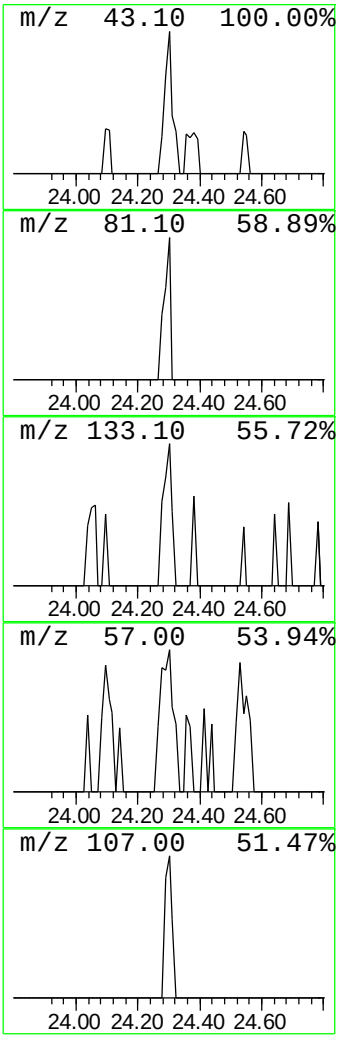
****

Peak Number 9 unknown24.30 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.30	2.48 ng	28890	Perylene-d12	22.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 4-(2,6,6-trimethyl...	194	C13H22O	022029-76-1	38
2	.beta.-Panasinsene	204	C15H24	1000159-39-0	38
3	Cedran-diol, 8S,14-	238	C15H26O2	062600-05-9	35
4	Ledene oxide-(II)	220	C15H24O	1000159-36-7	35
5	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077049.D
Acq On : 26 Jan 2015 12:19
Operator : TP/IZ
Sample : PB81273BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB81273BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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...	3.83	25.0	ng	179606	1	7.76	143941	20.0
unknown7.25	7.25	100.7	ng	724663	1	7.76	143941	20.0
Hexadecanoic acid...	19.79	6.0	ng	76563	5	21.13	254022	20.0
Octadecanoic acid...	20.68	4.0	ng	51411	5	21.13	254022	20.0
unknown24.30	24.30	2.5	ng	28890	6	22.78	232777	20.0