LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

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-BF090115.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	4.318	237	239	241	rBV	13540	21958	1.12%	0.147%
2	4.375	241	244	256	rVB	469179	842167	42.88%	5.621%
3	4.570	256	261	265	rBV	9307	28611	1.46%	0.191%
4	4.890	286	289	291	rBV	1018474	1366984	69.61%	9.123%
5	6.010	384	387	389	rBV	1579233	1690791	86.09%	11.284%
6	6.101	393	395	397	rVV	1556834	1467984	74.75%	9.797%
7	6.216	400	405	411	rVV	50148	145551	7.41%	0.971%
8	6.330	413	415	418	rVB	443670	374650	19.08%	2.500%
9	6.490	426	429	431	rBV	1320921	1322781	67.36%	8.828%
10	6.913	463	466	468	rBV	1115412	1121627	57.11%	7.486%
11	7.622	526	528	530	rBV	542681	468827	23.87%	3.129%
12	8.707	620	623	625	rBV	2161273	1963887	100.00%	13.107%
13	9.107	656	658	660	rBV	211162	178584	9.09%	1.192%
14	9.359	678	680	683	rVB	544933	471875	24.03%	3.149%
15	9.793	713	718	720	rBV3	10698	26501	1.35%	0.177%
16	10.136	746	748	751	rBV2	211495	276276	14.07%	1.844%
17	10.296	758	762	765	rBV2	34659	44888	2.29%	0.300%
18	10.742	799	801	802	rBV	27330	28974	1.48%	0.193%
19	10.822	806	808	811	rVV	529886	470904	23.98%	3.143%
20	12.411	944	947	949	rBV	1741403	1640818	83.55%	10.951%
21	13.325	1025	1027	1034	rVB	159409	198289	10.10%	1.323%
22	13.428	1034	1036	1041	rBV	438584	420684	21.42%	2.808%
23	13.645	1053	1055	1061	rBV3	11603	20749	1.06%	0.138%
24	13.954	1080	1082	1086	rBV	18165	27028	1.38%	0.180%
25	14.731	1148	1150	1153	rBV	247105	270289	13.76%	1.804%
26	15.154	1185	1187	1195	rVB2	27561	54867	2.79%	0.366%
27	15.954	1254	1257	1267	rVB6	9913	37270	1.90%	0.249%

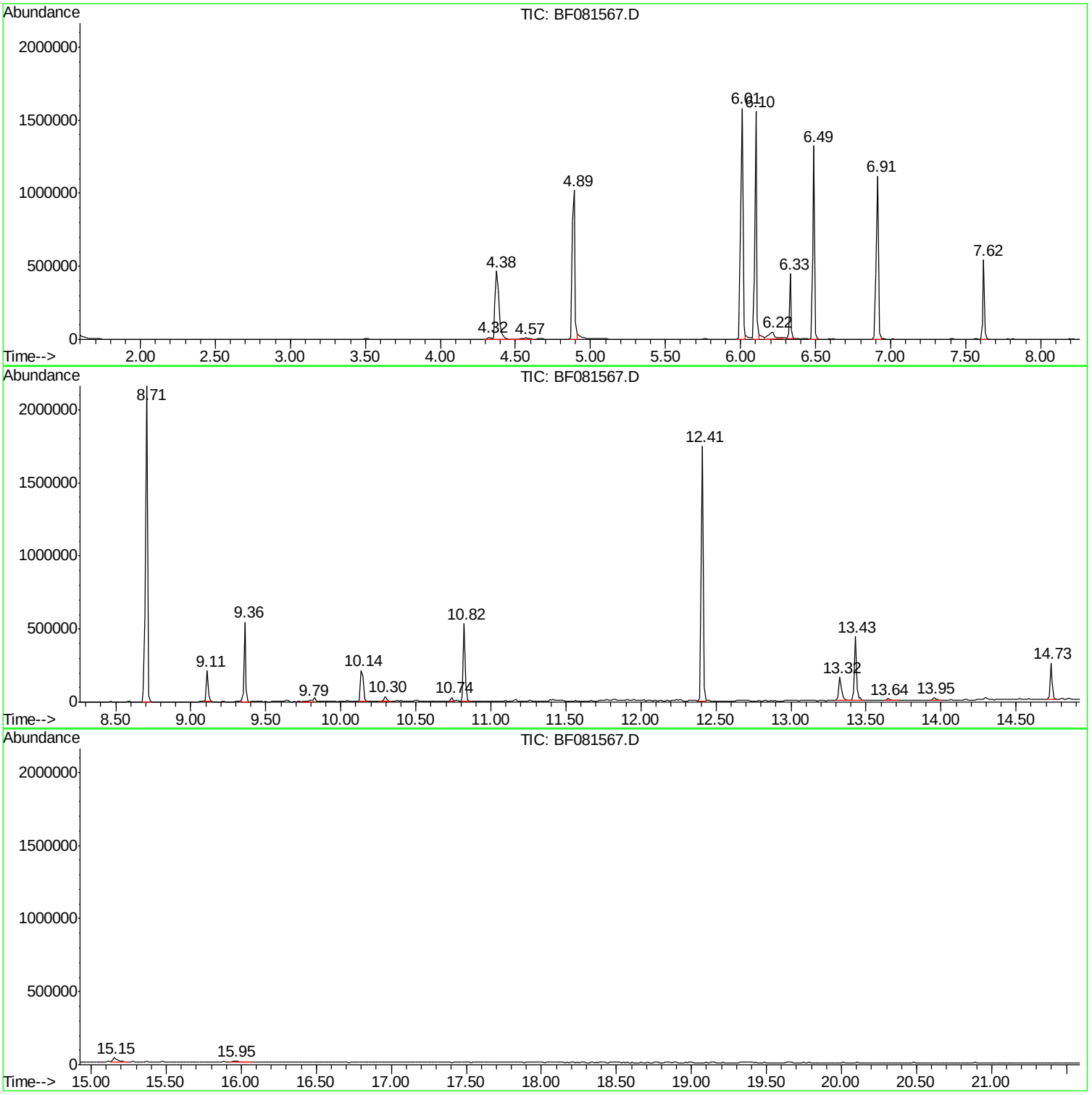
Sum of corrected areas: 14983814

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

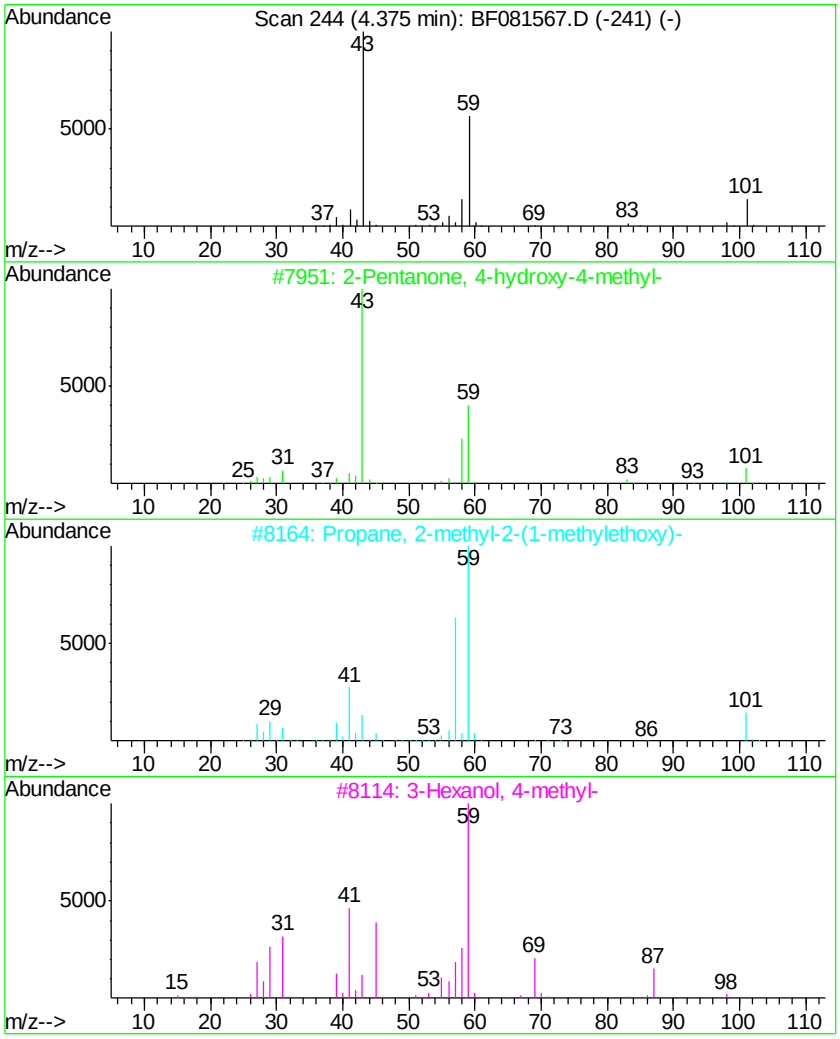
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

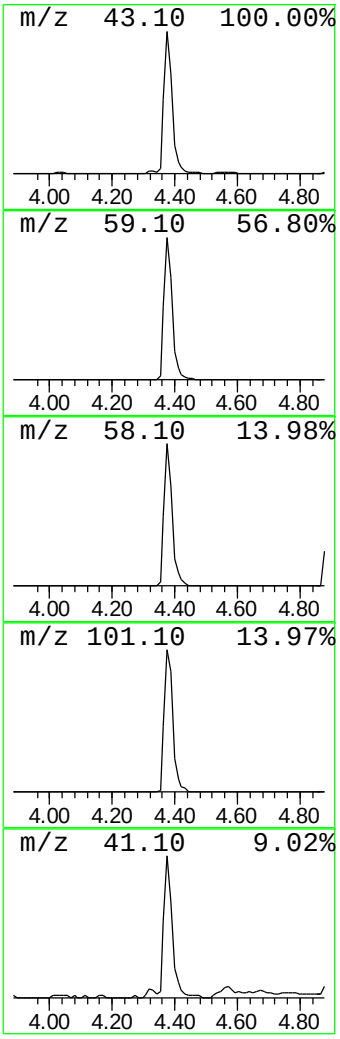
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	44.96 ng	842167	1,4-Dichlorobenzene-d4	6.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

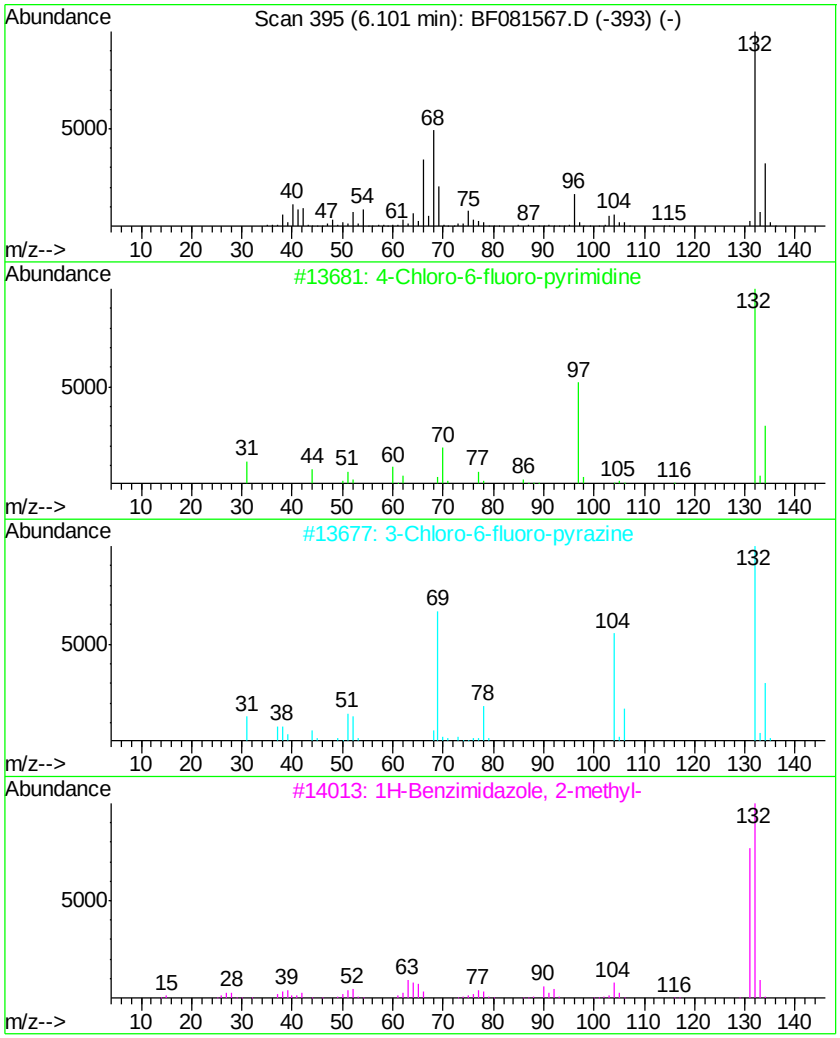
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

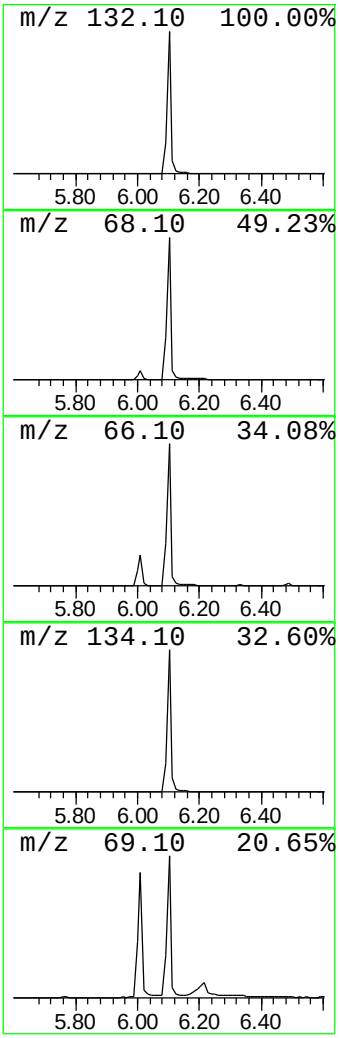
****

Peak Number 2 unknown6.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.10	78.37 ng	1467980	1,4-Dichlorobenzene-d4	6.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

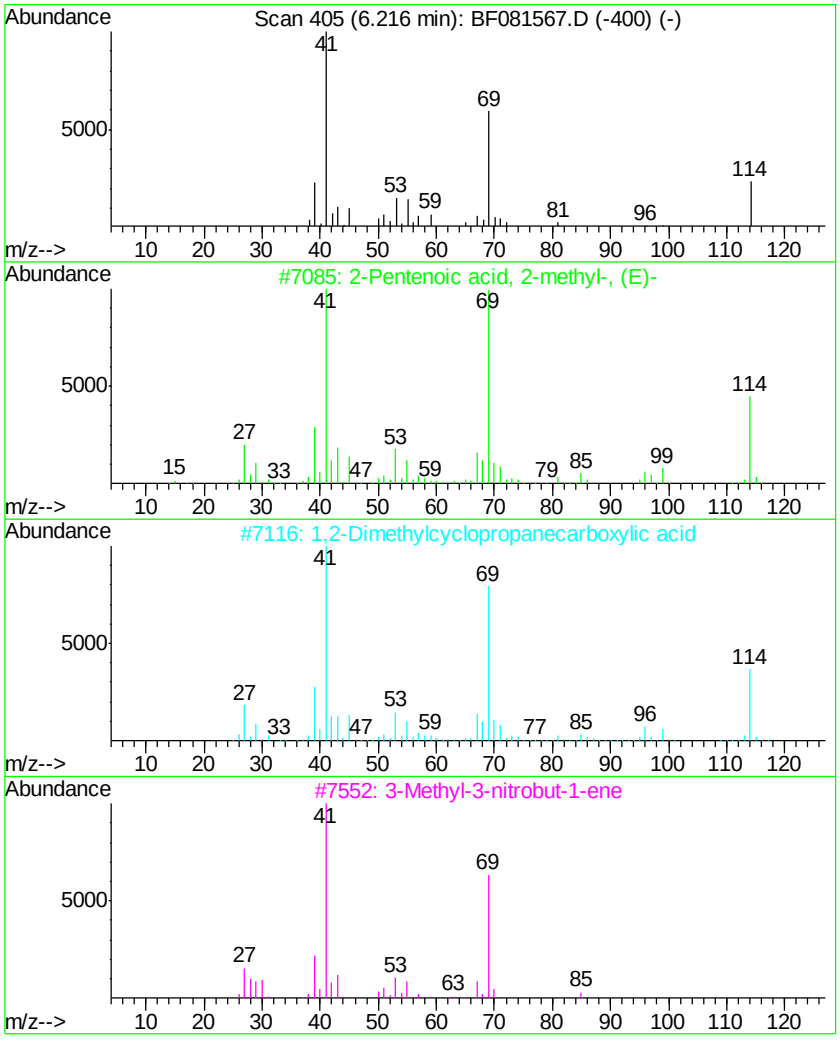
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

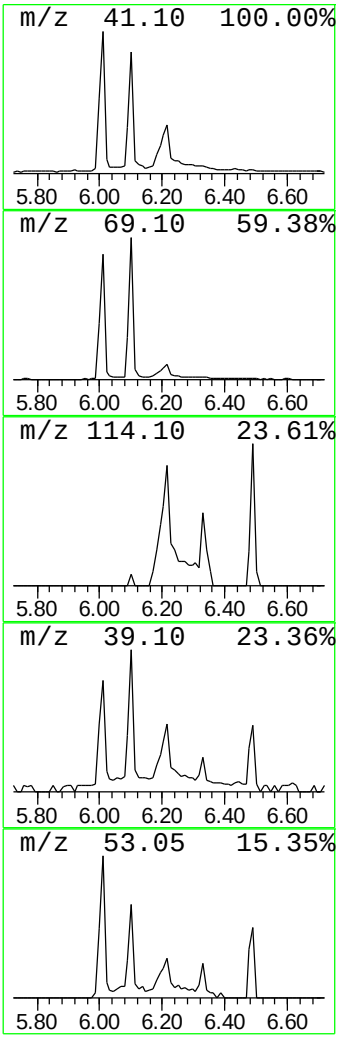
****

Peak Number 3 unknown6.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	7.77 ng	145551	1,4-Dichlorobenzene-d4	6.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenoic acid, 2-methyl-, (E)-	114	C6H10O2	016957-70-3	42
2	1,2-Dimethylcyclopropanecarboxyl...	114	C6H10O2	1000191-14-6	40
3	3-Methyl-3-nitrobut-1-ene	115	C5H9NO2	001809-67-2	38
4	Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	23
5	3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

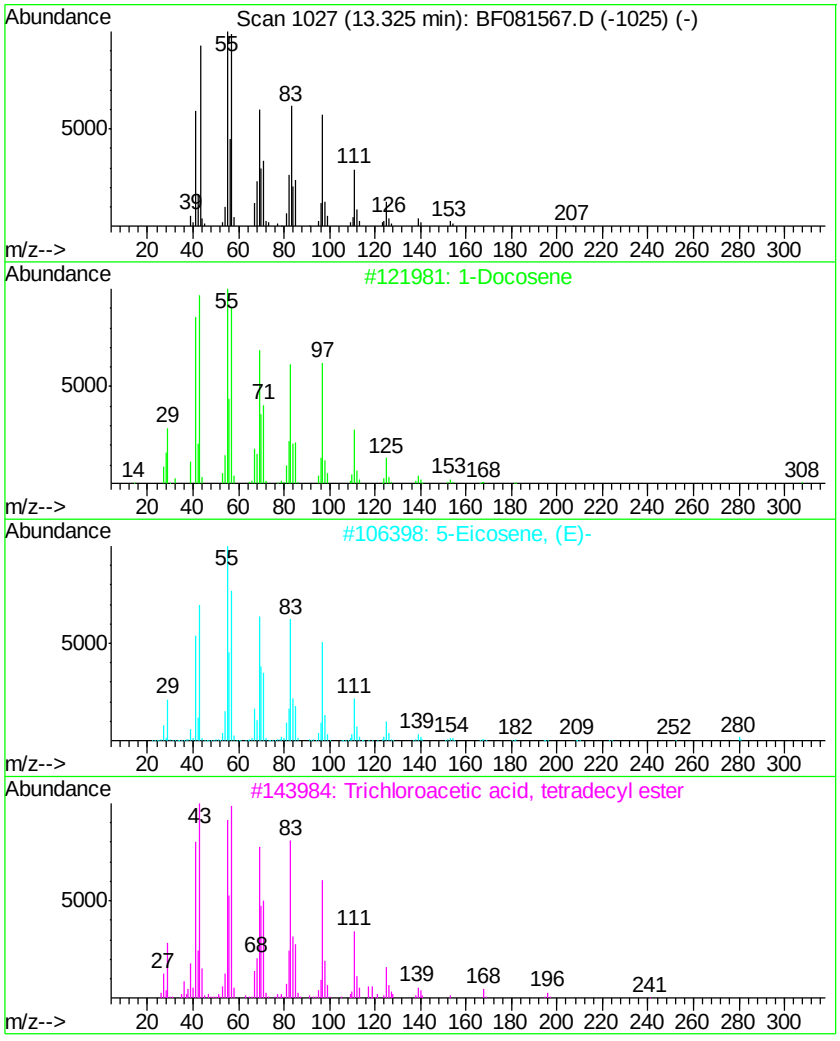
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

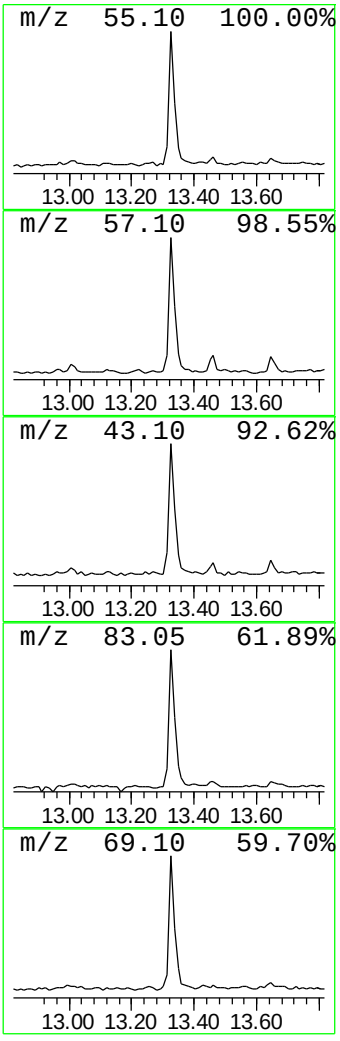
****

Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	9.43 ng	198289	Chrysene-d12	13.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
4	1-Pentadecanol	228	C15H32O	000629-76-5	83
5	1-Tetracosanol	354	C24H50O	000506-51-4	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

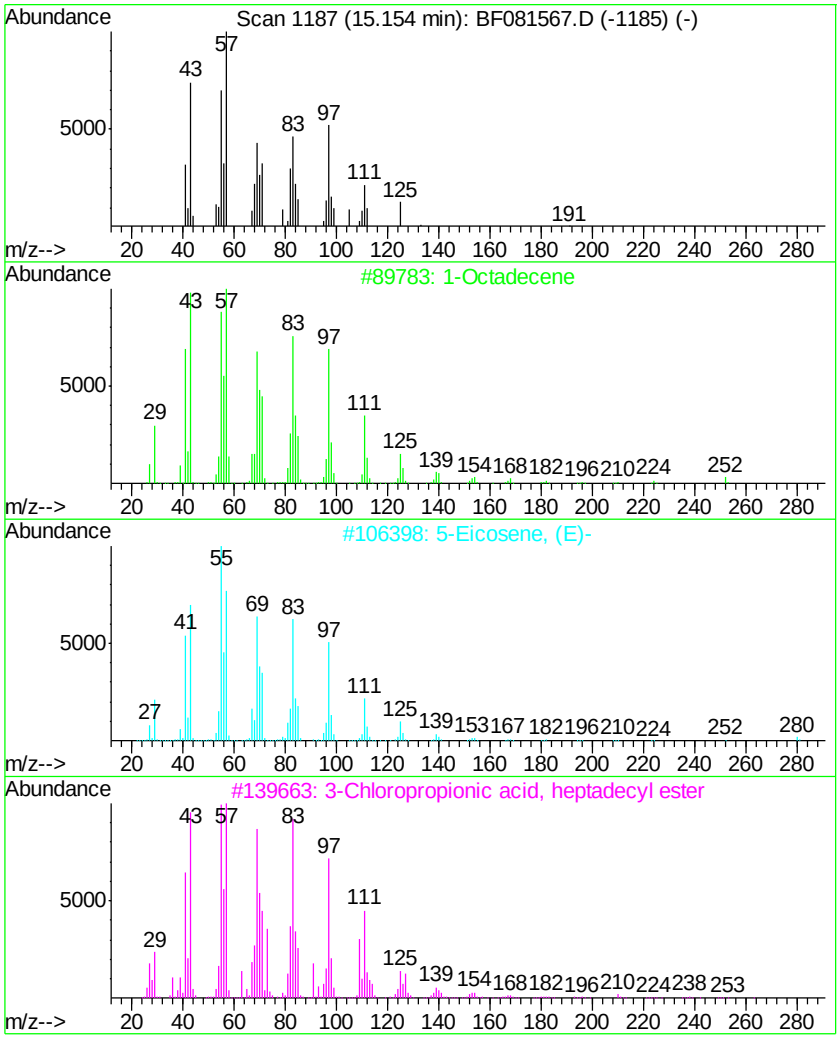
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

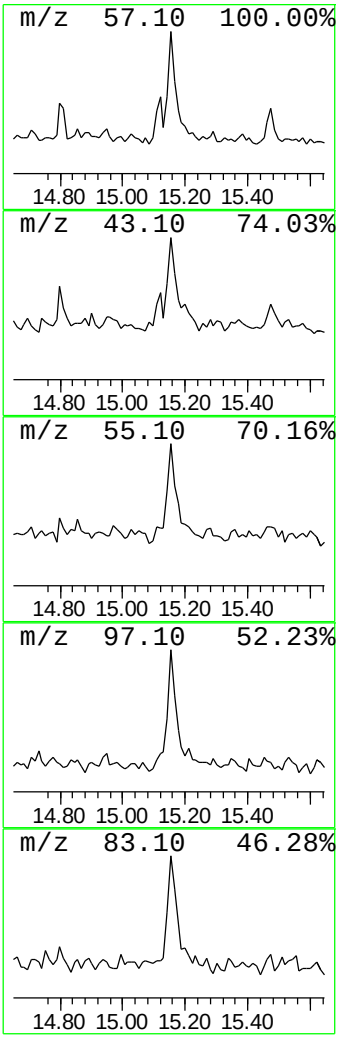
****

Peak Number 6 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	4.06 ng	54867	Perylene-d12	14.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
4	1-Eicosanol	298	C20H42O	000629-96-9	74
5	1-Heptadecene	238	C17H34	006765-39-5	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

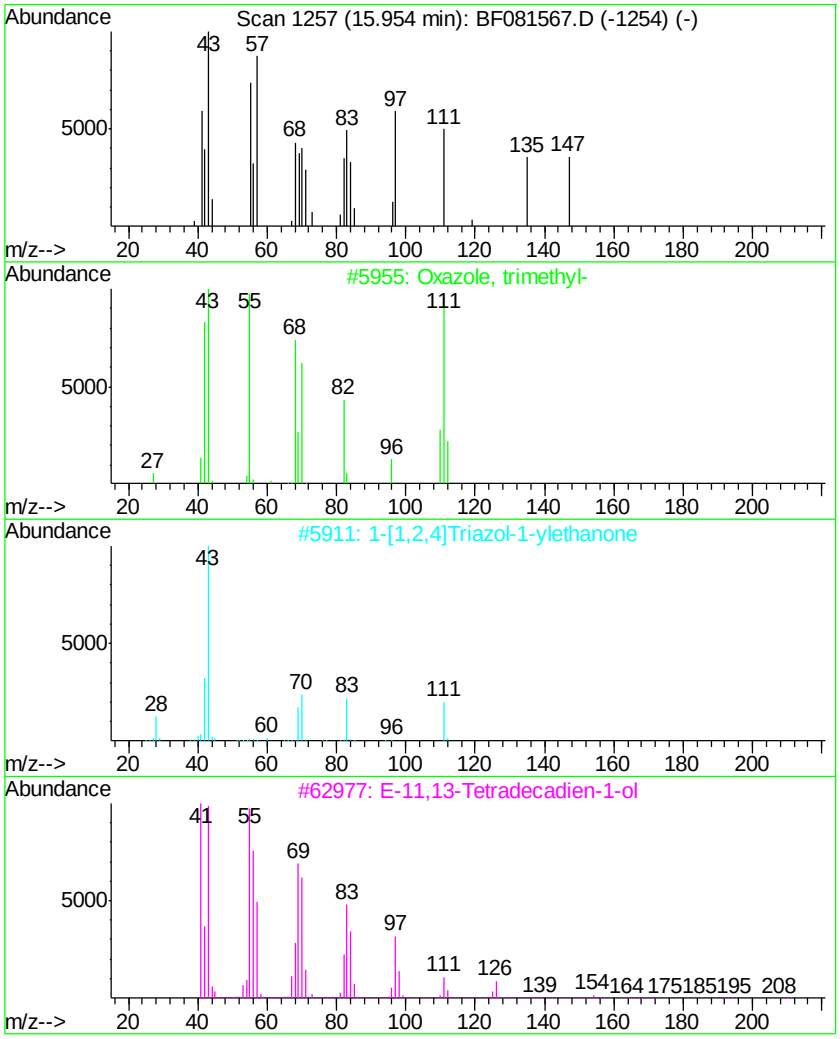
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

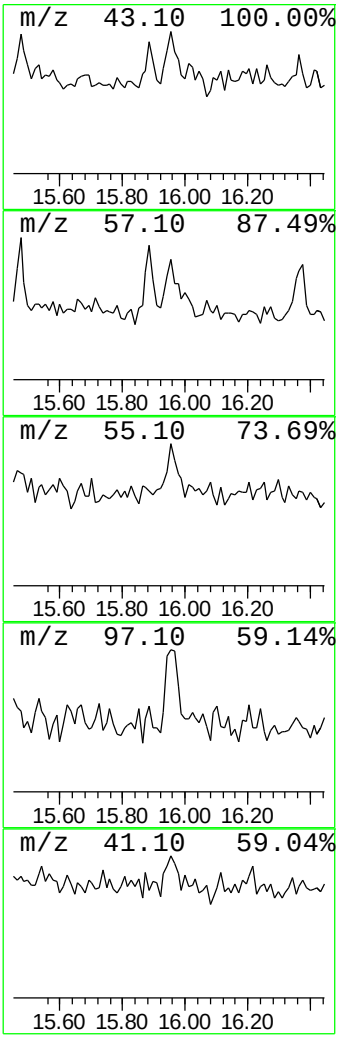
****

Peak Number 7 unknown15.95 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	2.76 ng	37270	Perylene-d12	14.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole, trimethyl-	111	C6H9NO	020662-84-4	43
2	1-[1,2,4]Triazol-1-ylethanone	111	C4H5N3O	015625-88-4	38
3	E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	38
4	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	38
5	1-Docosene	308	C22H44	001599-67-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090915\
Data File : BF081567.D
Acq On : 9 Sep 2015 22:50
Operator : UM/IZ
Sample : G3582-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-I-8-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.38	45.0	ng	842167	1	6.33	374650	20.0
unknown6.10	6.10	78.4	ng	1467980	1	6.33	374650	20.0
unknown6.22	6.22	7.8	ng	145551	1	6.33	374650	20.0
1-Docosene	13.32	9.4	ng	198289	5	13.43	420684	20.0
1-Octadecene	15.15	4.1	ng	54867	6	14.73	270289	20.0
unknown15.95	15.95	2.8	ng	37270	6	14.73	270289	20.0