LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081715\
Data File : BF081011.D
Acq On : 17 Aug 2015 19:14
Operator : UM/IZ
Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

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-BF081715.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	4.021	175	178	184	rBV	45400	69316	3.42%	0.377%
2	4.753	238	242	245	rBV	843091	1572577	77.59%	8.562%
3	5.199	278	281	284	rBV	1438990	1652470	81.53%	8.997%
4	5.622	315	318	320	rBV	62484	56393	2.78%	0.307%
5	6.273	371	375	377	rBV	1779549	2026756	100.00%	11.035%
6	6.387	383	385	388	rBV	1505087	1583307	78.12%	8.621%
7	6.627	403	406	408	rBV	534769	494225	24.39%	2.691%
8	6.776	417	419	422	rBV	947325	1180444	58.24%	6.427%
9	7.199	453	456	458	rBV	935690	1228435	60.61%	6.689%
10	7.907	516	518	521	rBV	660014	621218	30.65%	3.382%
11	8.993	610	613	615	rBV	1853281	1766227	87.15%	9.617%
12	9.393	645	648	650	rBV	295732	346797	17.11%	1.888%
13	9.656	669	671	674	rBB	747786	669329	33.02%	3.644%
14	10.445	737	740	742	rVB	901019	1097654	54.16%	5.976%
15	10.582	750	752	755	rBV	32086	44918	2.22%	0.245%
16	11.028	788	791	792	rBV	31487	34179	1.69%	0.186%
17	11.131	797	800	802	rVV	884936	745666	36.79%	4.060%
18	11.451	826	828	830	rVB	31377	28165	1.39%	0.153%
19	11.679	846	848	850	rBV	28694	27127	1.34%	0.148%
20	12.559	923	925	926	rBV	21508	21980	1.08%	0.120%
21	12.719	936	939	941	rBV	1639601	1737855	85.75%	9.462%
22	13.257	984	986	989	rBV	18523	20526	1.01%	0.112%
23	13.634	1017	1019	1027	rBV2	32716	85200	4.20%	0.464%
24	13.748	1027	1029	1031	rBV	747255	674085	33.26%	3.670%
25	14.514	1094	1096	1100	rBV2	57167	82124	4.05%	0.447%
26	14.605	1102	1104	1109	rVB	29196	31095	1.53%	0.169%
27	15.097	1144	1147	1150	rBV	403813	468306	23.11%	2.550%

Sum of corrected areas: 18366374

LSC Report - Integrated Chromatogram

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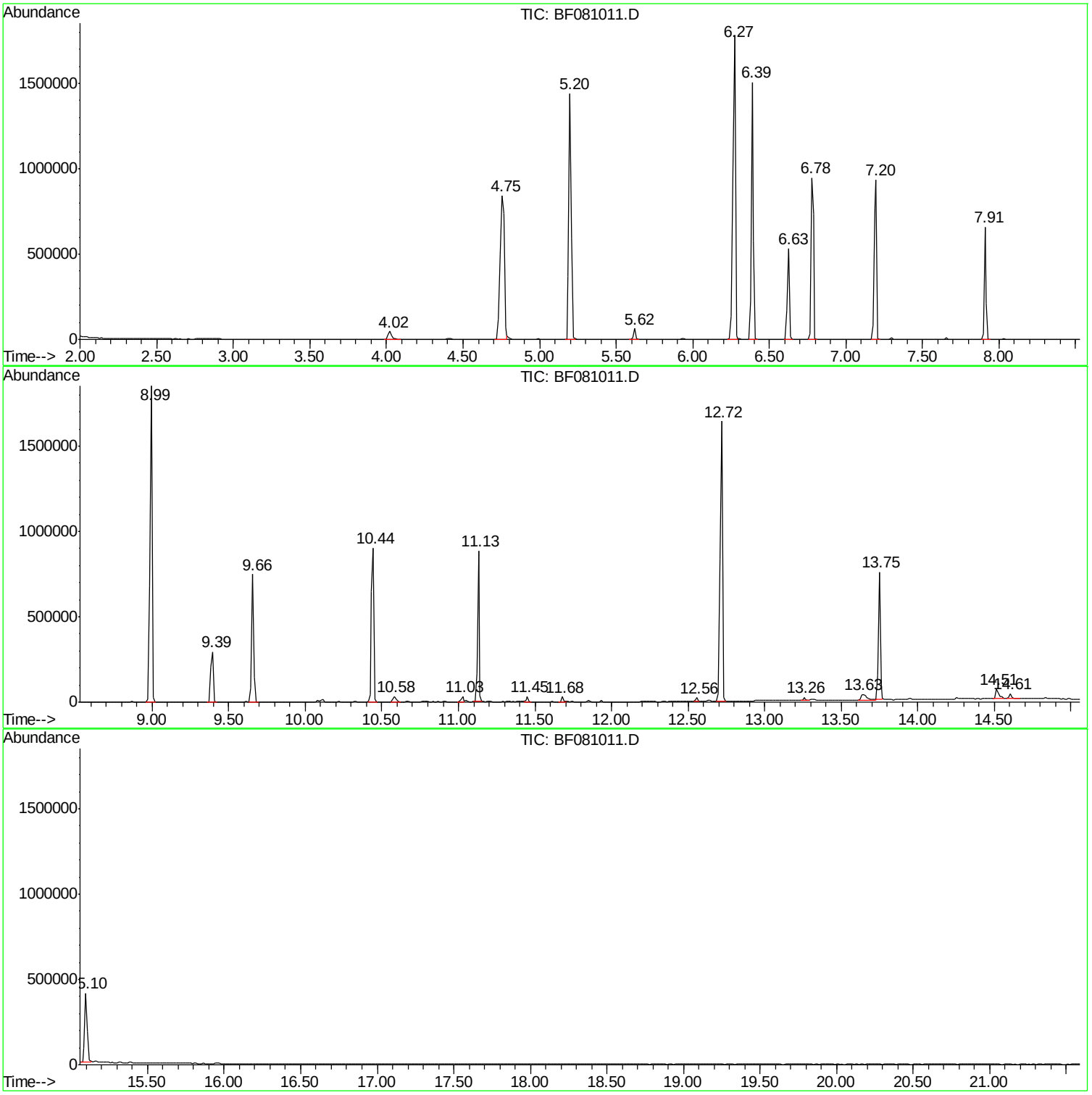
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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\BF081715\
Data File : BF081011.D
Acq On : 17 Aug 2015 19:14
Operator : UM/IZ
Sample : G3282-16
Misc :
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Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

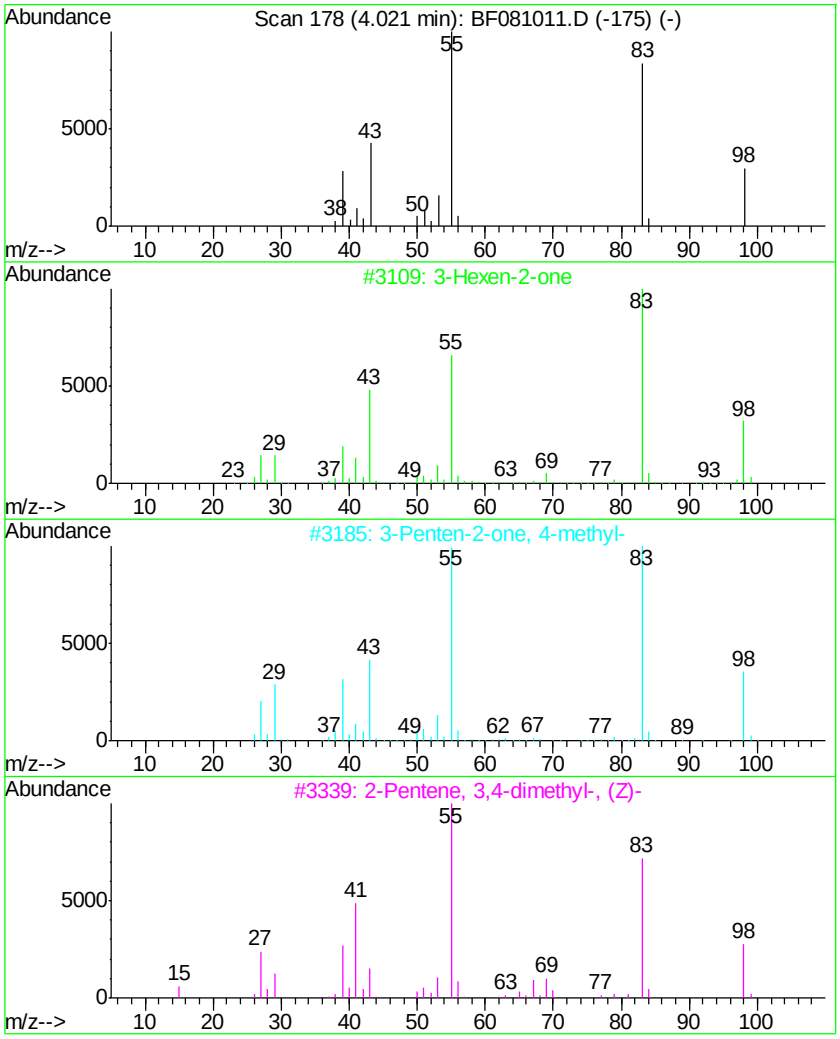
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

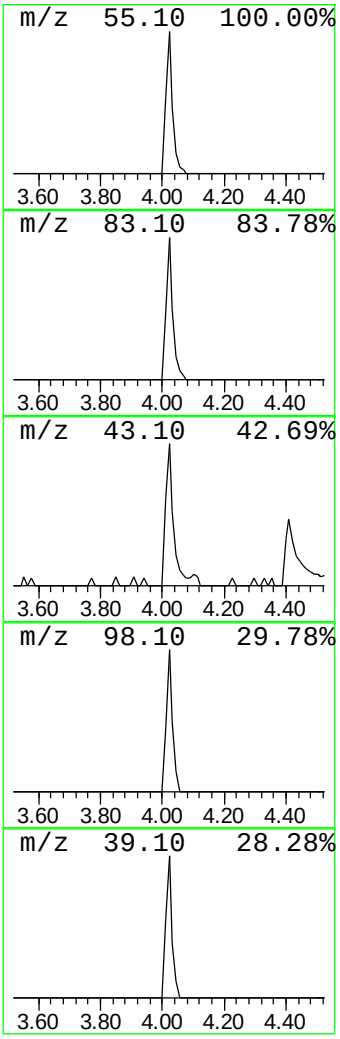
****

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	2.81 ng	69316	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	86
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081715\
Data File : BF081011.D
Acq On : 17 Aug 2015 19:14
Operator : UM/IZ
Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

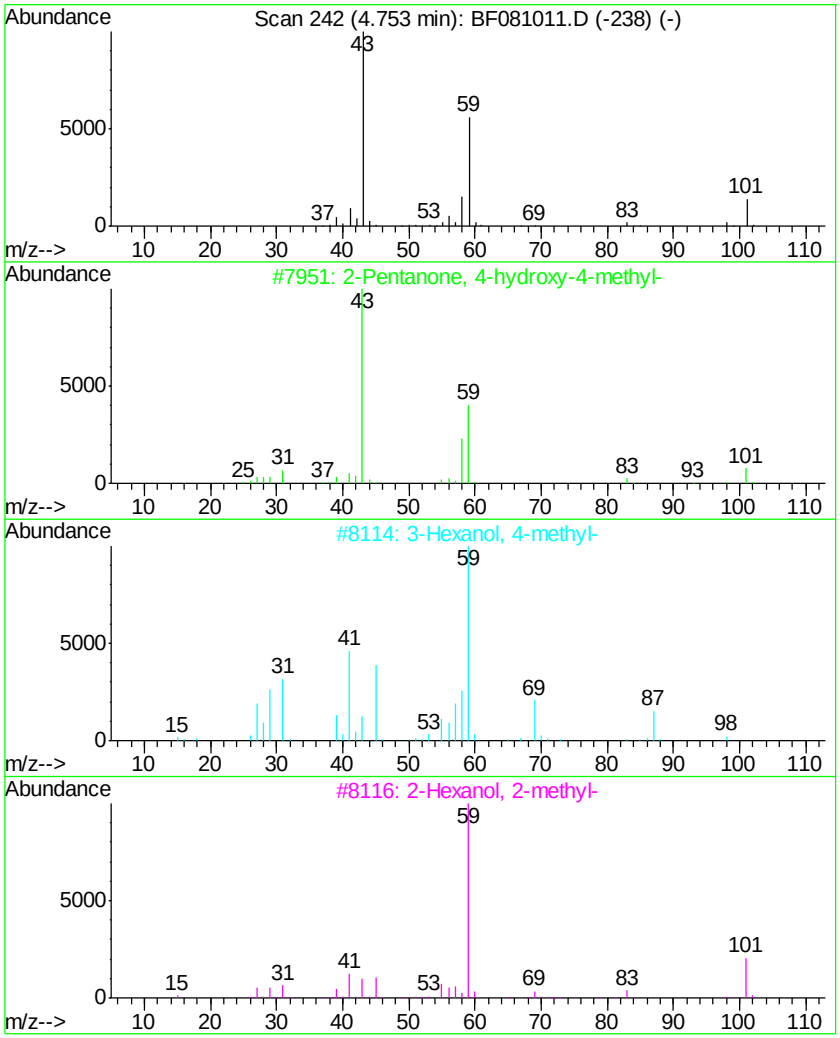
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

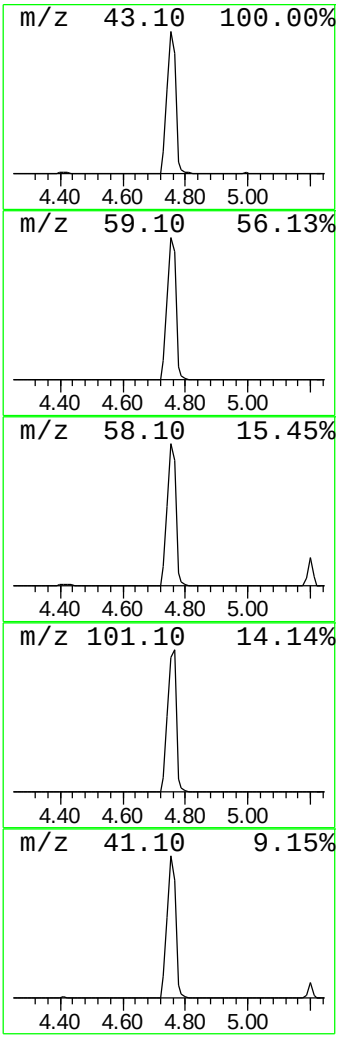
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	63.64 ng	1572580	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081715\
Data File : BF081011.D
Acq On : 17 Aug 2015 19:14
Operator : UM/IZ
Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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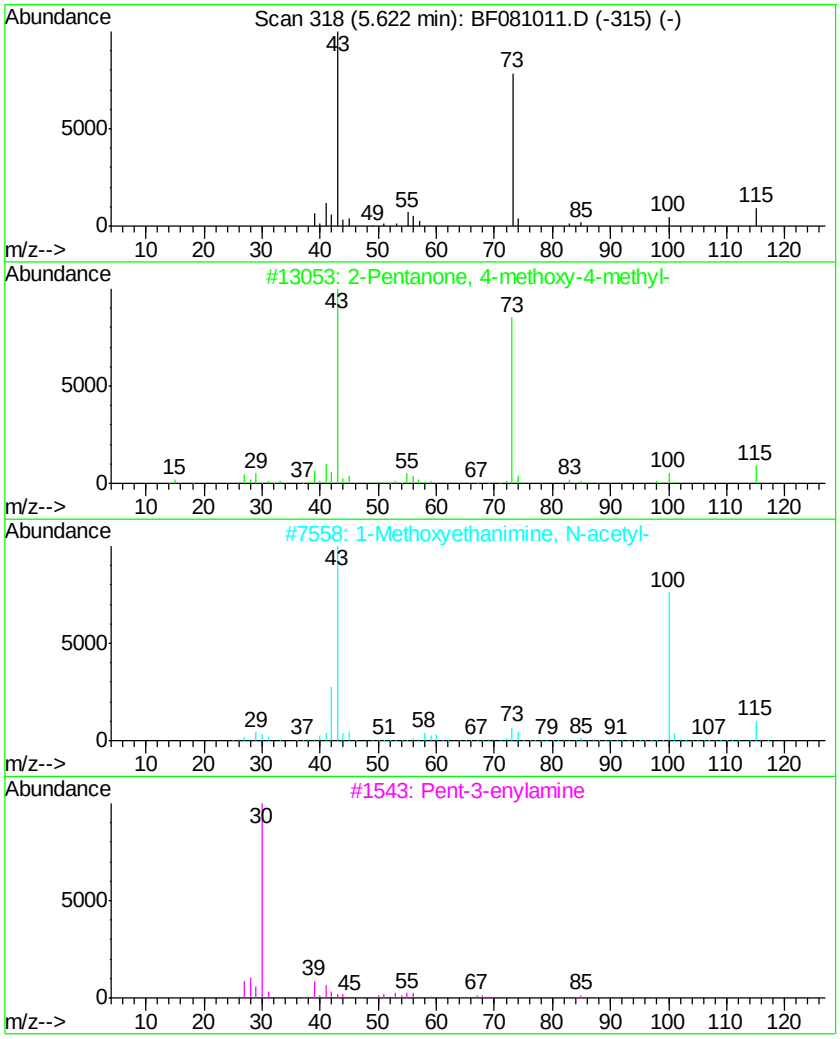
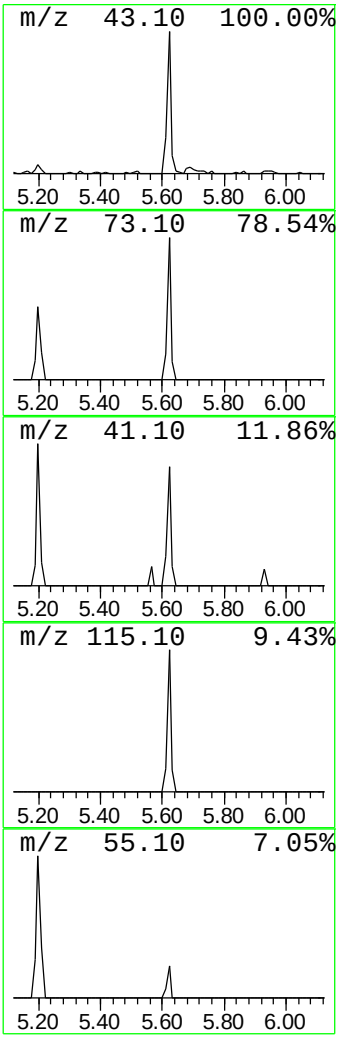
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.62	2.28 ng	56393	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
3	Pent-3-enylamine	85	C5H11N	087156-70-5	9
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





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Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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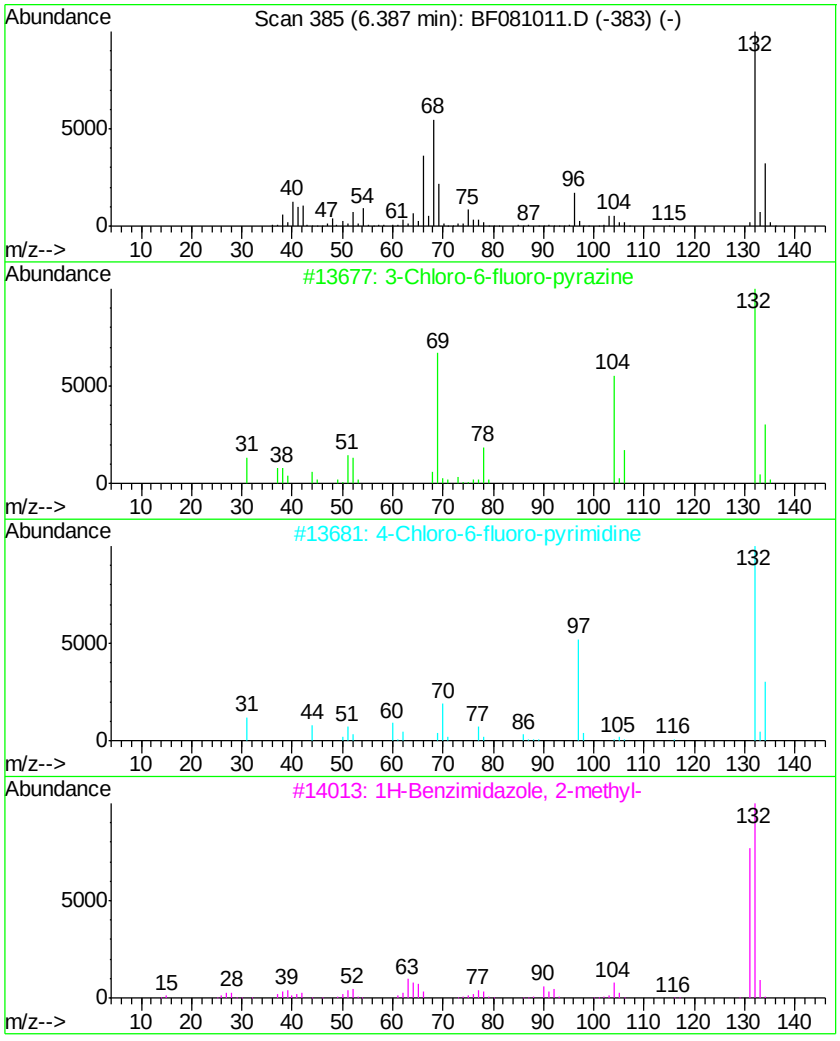
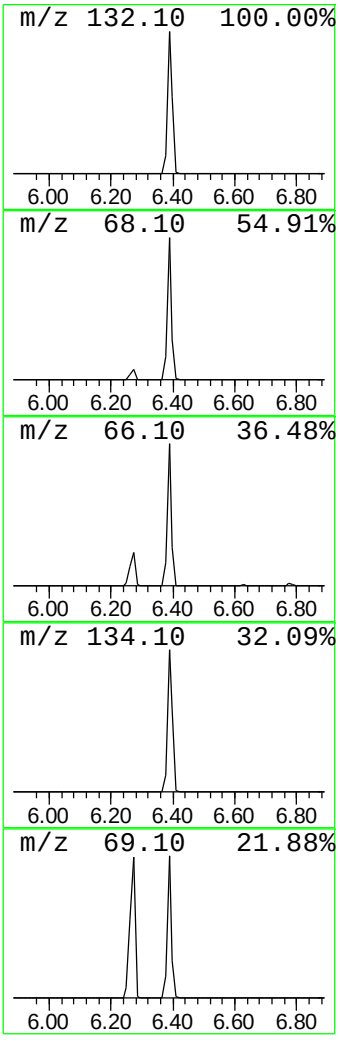
Peak Number 4 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	64.07 ng	1583310	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Operator : UM/IZ
Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

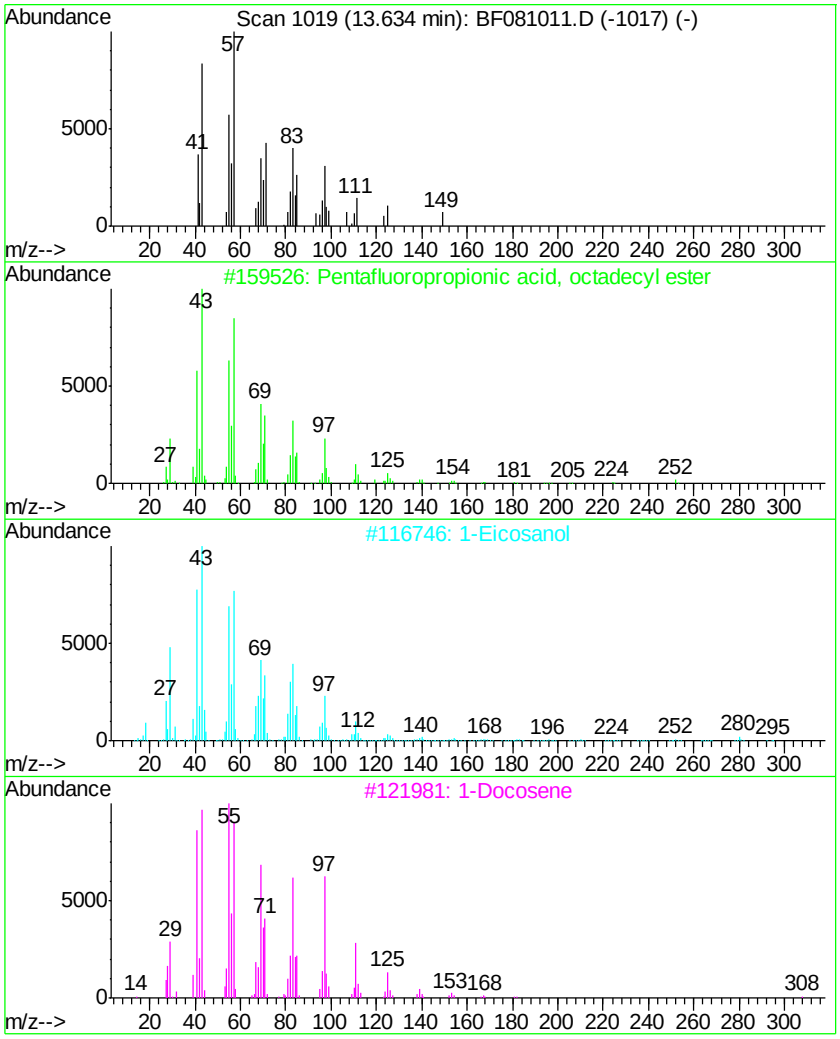
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

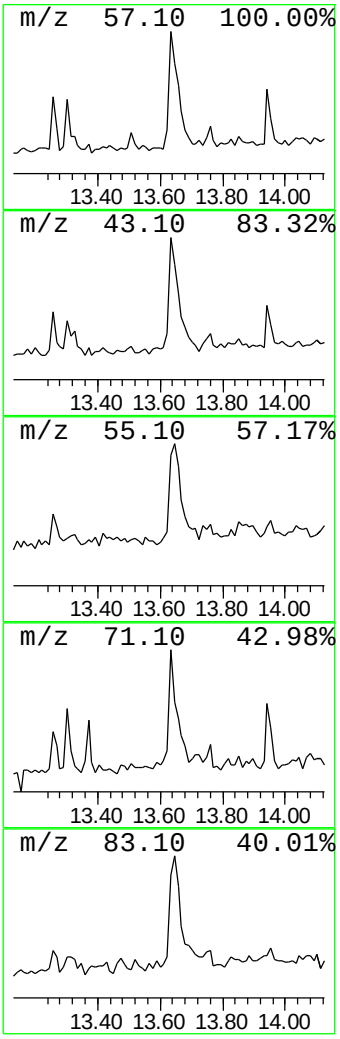
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.53 ng	85200	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2	1-Eicosanol	298	C20H42O	000629-96-9	90
3	1-Docosene	308	C22H44	001599-67-3	72
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
5	1-Nonadecanol	284	C19H40O	001454-84-8	72





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Sample : G3282-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB06-1.0-2.0-081215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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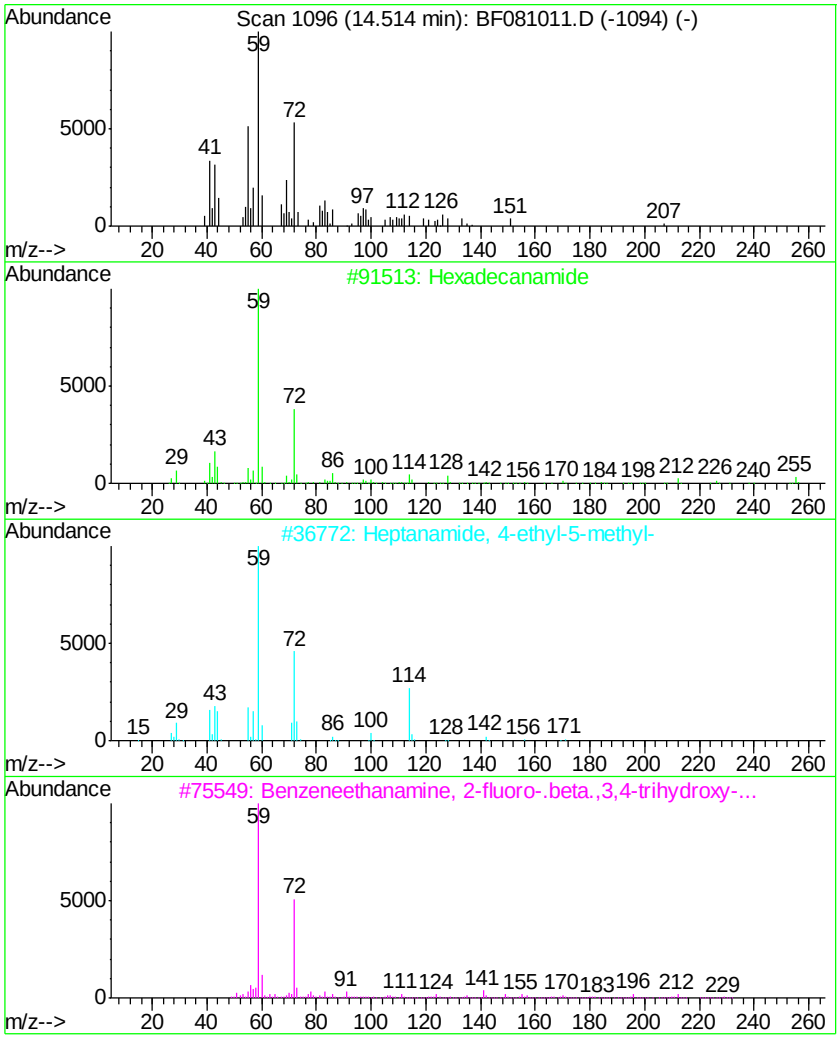
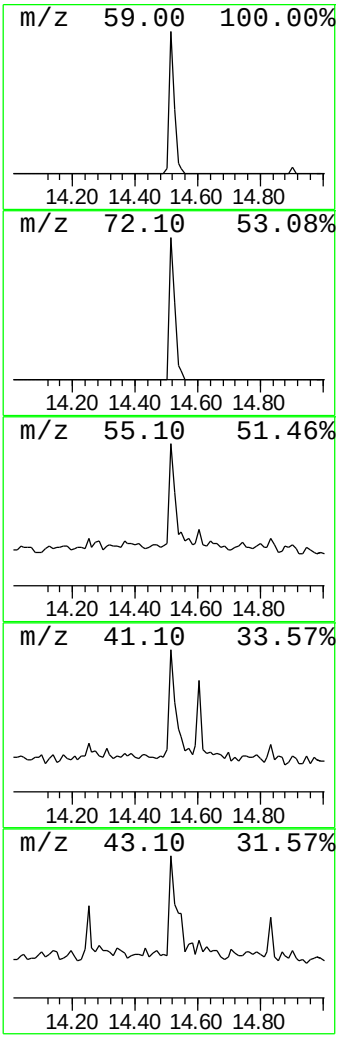
Peak Number 7 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	3.51 ng	82124	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	64
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
4	Nonanamide	157	C9H19NO	001120-07-6	50
5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	43





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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
3-Hexen-2-one	4.02	2.8	ng	69316	1	6.63	494225	20.0
2-Pentanone, 4-hy...	4.75	63.6	ng	1572580	1	6.63	494225	20.0
2-Pentanone, 4-me...	5.62	2.3	ng	56393	1	6.63	494225	20.0
unknown6.39	6.39	64.1	ng	1583310	1	6.63	494225	20.0
Pentafluoropropio...	13.63	2.5	ng	85200	5	13.75	674085	20.0
Hexadecanamide	14.51	3.5	ng	82124	6	15.10	468306	20.0