LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081278.D
Acq On : 29 Aug 2015 18:52
Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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	4.560	245	247	257	rVB	328400	466796	31.77%	3.669%
2	5.040	286	289	296	rBV	884280	909326	61.89%	7.147%
3	6.126	382	384	387	rBV	469641	575561	39.17%	4.524%
4	6.240	392	394	397	rVB	964871	1186398	80.74%	9.325%
5	6.480	412	415	417	rBV	425071	369904	25.17%	2.907%
6	6.640	426	429	431	rBV	889493	1084118	73.78%	8.521%
7	7.052	463	465	468	rBV	910331	877805	59.74%	6.899%
8	7.520	504	506	509	rBV	20240	23744	1.62%	0.187%
9	7.703	518	522	526	rBV2	174330	289626	19.71%	2.276%
10	7.772	526	528	530	rVB	403566	476554	32.43%	3.746%
11	8.846	620	622	625	rBV	1354681	1469375	100.00%	11.549%
12	9.246	655	657	658	rBV	36215	41933	2.85%	0.330%
13	9.292	658	661	664	rVV	69748	150996	10.28%	1.187%
14	9.349	664	666	674	rVB2	11414	33352	2.27%	0.262%
15	9.509	678	680	683	rVB	604403	507078	34.51%	3.986%
16	10.298	746	749	751	rBV	701410	895130	60.92%	7.036%
17	10.881	794	800	802	rBV	12037	15633	1.06%	0.123%
18	10.972	806	808	811	rBV	384453	499011	33.96%	3.922%
19	11.544	855	858	860	rBV	122504	128904	8.77%	1.013%
20	12.321	924	926	932	rBV	98639	102679	6.99%	0.807%
21	12.561	945	947	950	rBV	1216055	1436222	97.74%	11.289%
22	13.487	1026	1028	1031	rBV	17007	22018	1.50%	0.173%
23	13.590	1035	1037	1039	rBV	527430	466336	31.74%	3.665%
24	14.390	1103	1107	1109	rBV	11721	16817	1.14%	0.132%
25	14.675	1130	1132	1135	rVB	21829	20209	1.38%	0.159%
26	14.915	1150	1153	1155	rBV	283812	332453	22.63%	2.613%
27	14.973	1155	1158	1161	rVB	76204	99178	6.75%	0.780%
28	15.315	1185	1188	1191	rBV	77650	100922	6.87%	0.793%
29	15.693	1218	1221	1225	rBV	41000	63248	4.30%	0.497%
30	16.676	1303	1307	1311	rVB	15136	32183	2.19%	0.253%
31	18.036	1418	1426	1432	rBV2	8708	29264	1.99%	0.230%

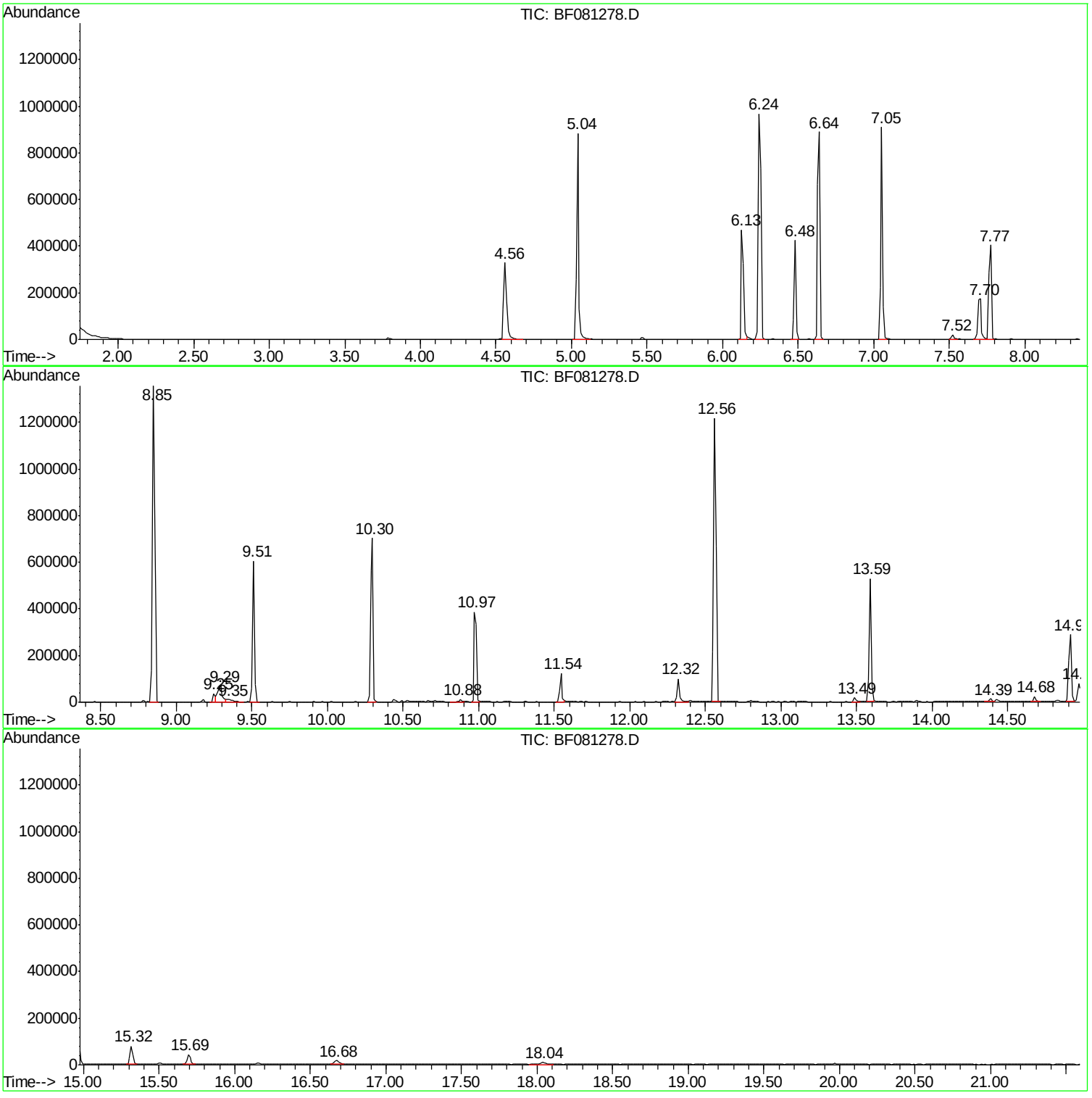
Sum of corrected areas: 12722773

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081278.D
Acq On : 29 Aug 2015 18:52
Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

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



Library Search Compound Report

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Operator : UM/IZ
Sample : G3467-04
Misc :
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Instrument : BNA_F
ClientSampleId : MW-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

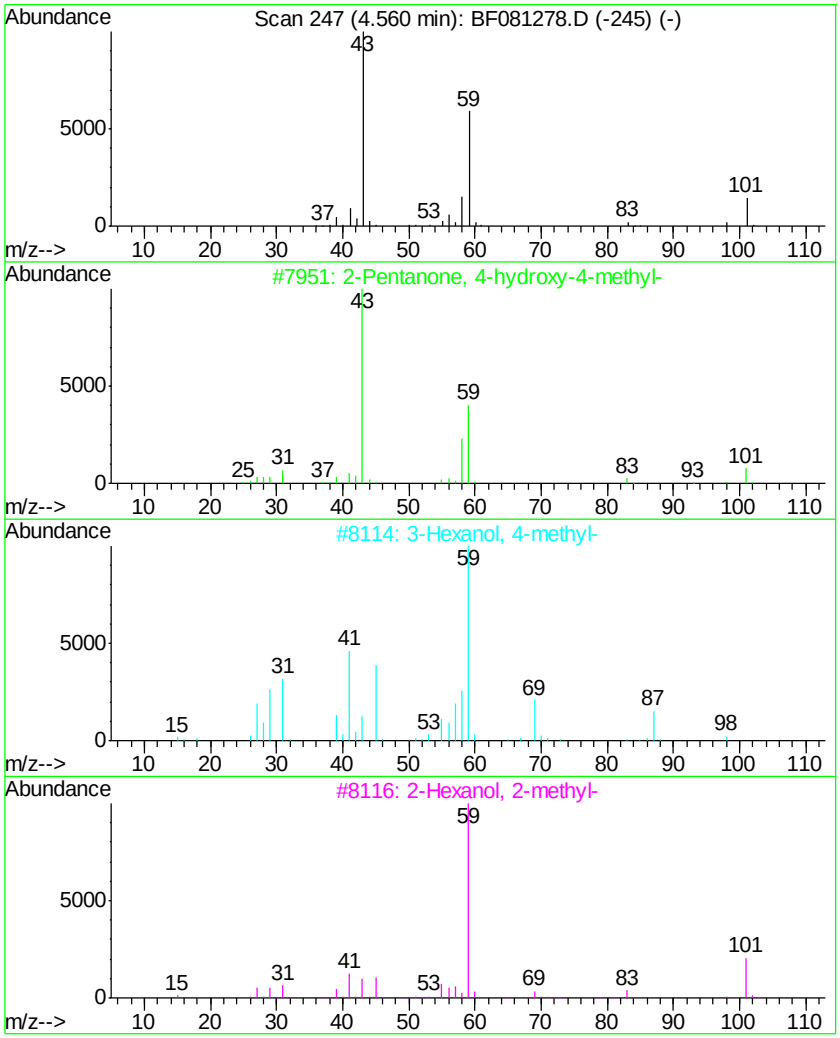
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

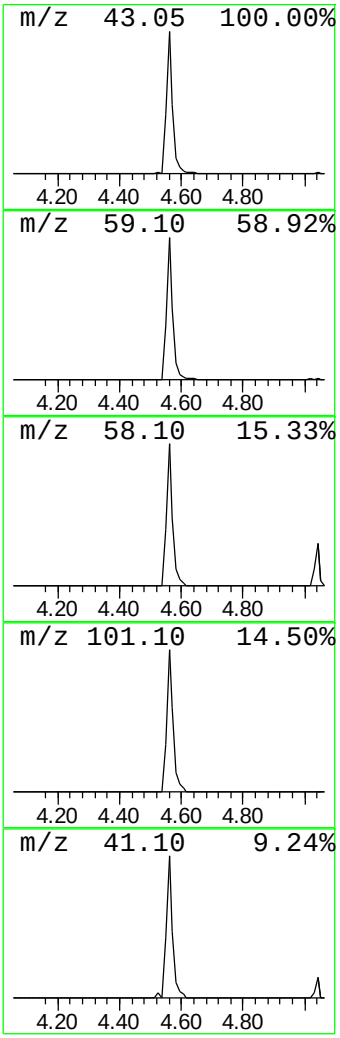
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	25.24 ng	466796	1,4-Dichlorobenzene-d4	6.48

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	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Data File : BF081278.D
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Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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

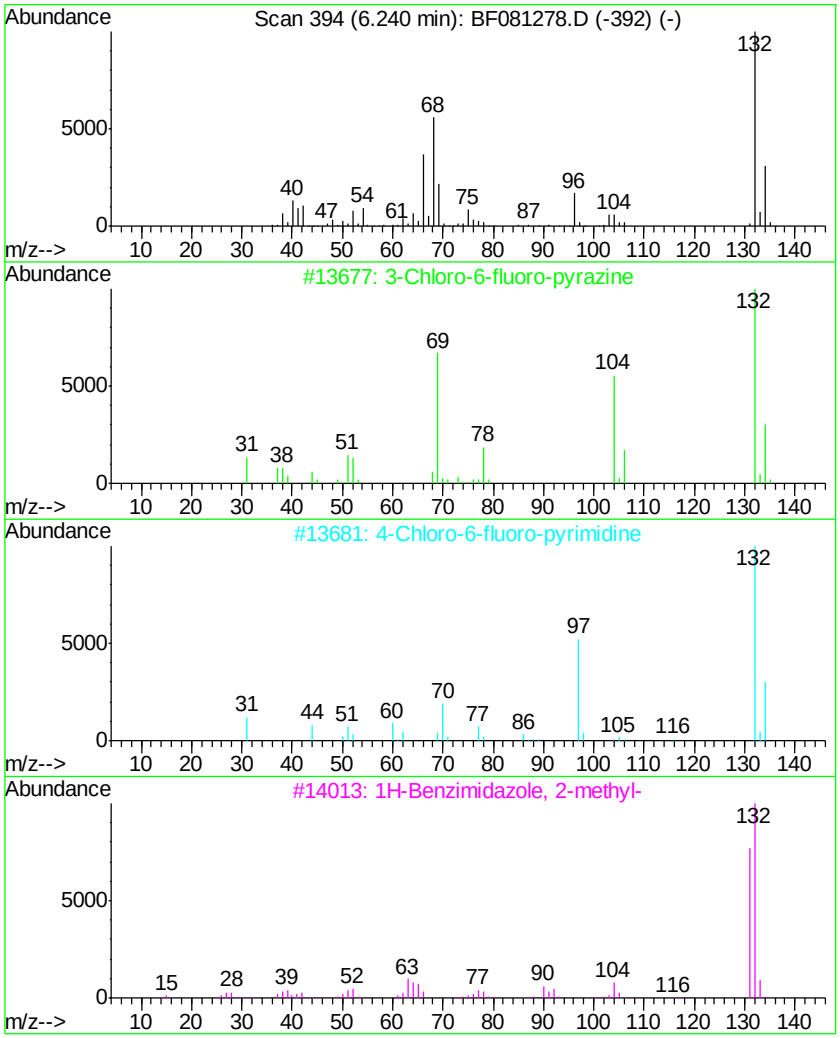
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

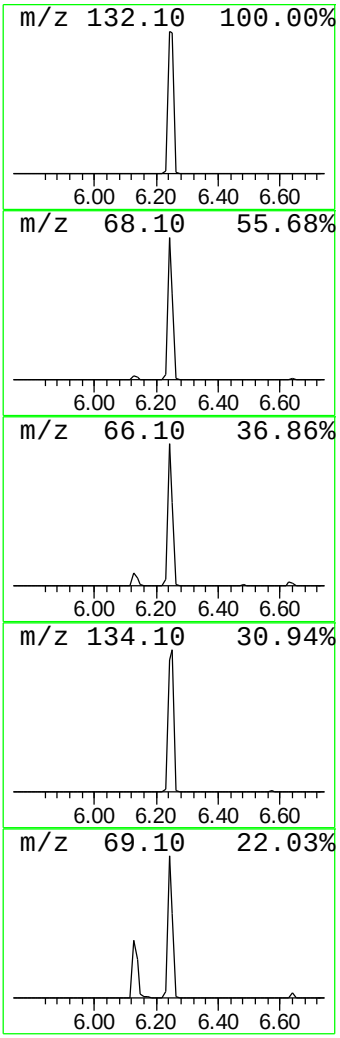
****

Peak Number 2 unknown6.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	64.15 ng	1186400	1,4-Dichlorobenzene-d4	6.48

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	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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
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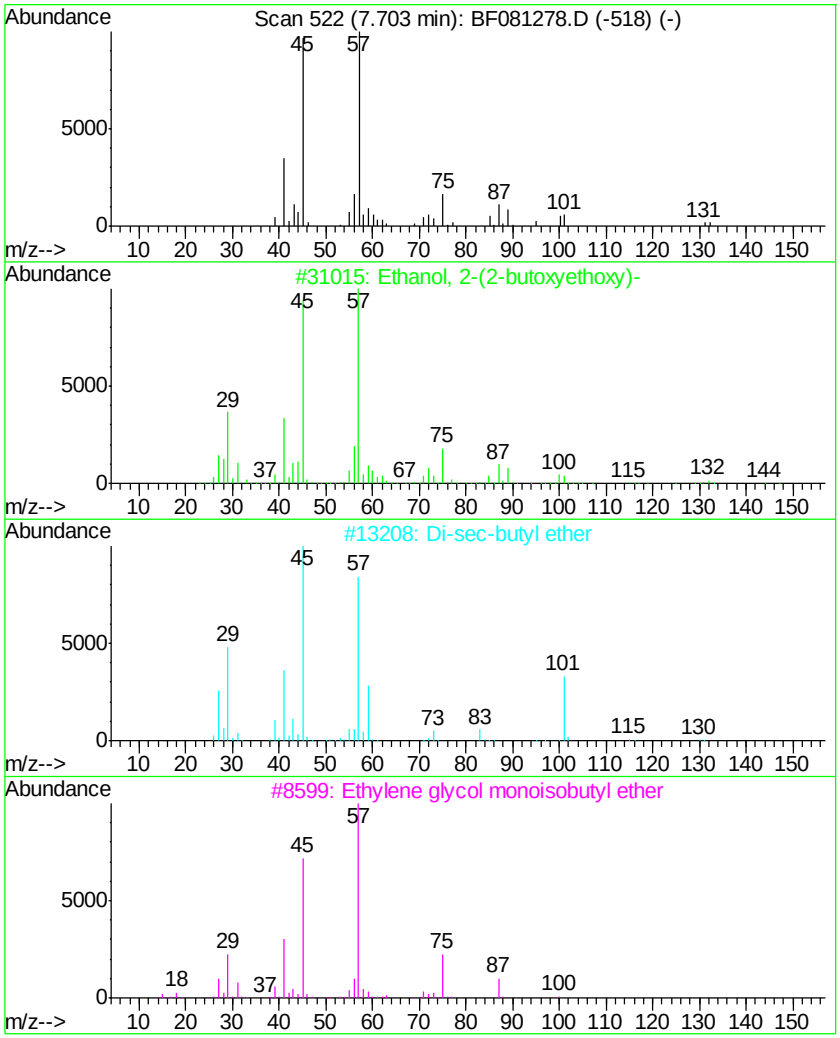
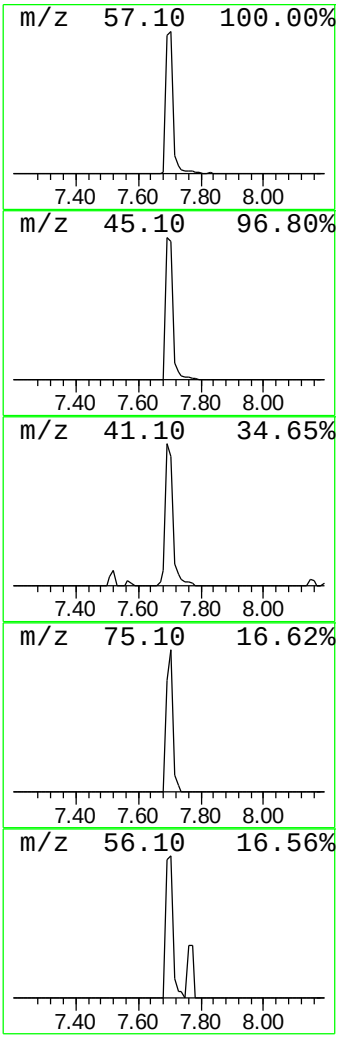
****

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	12.16 ng	289626	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	43





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Data File : BF081278.D
Acq On : 29 Aug 2015 18:52
Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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

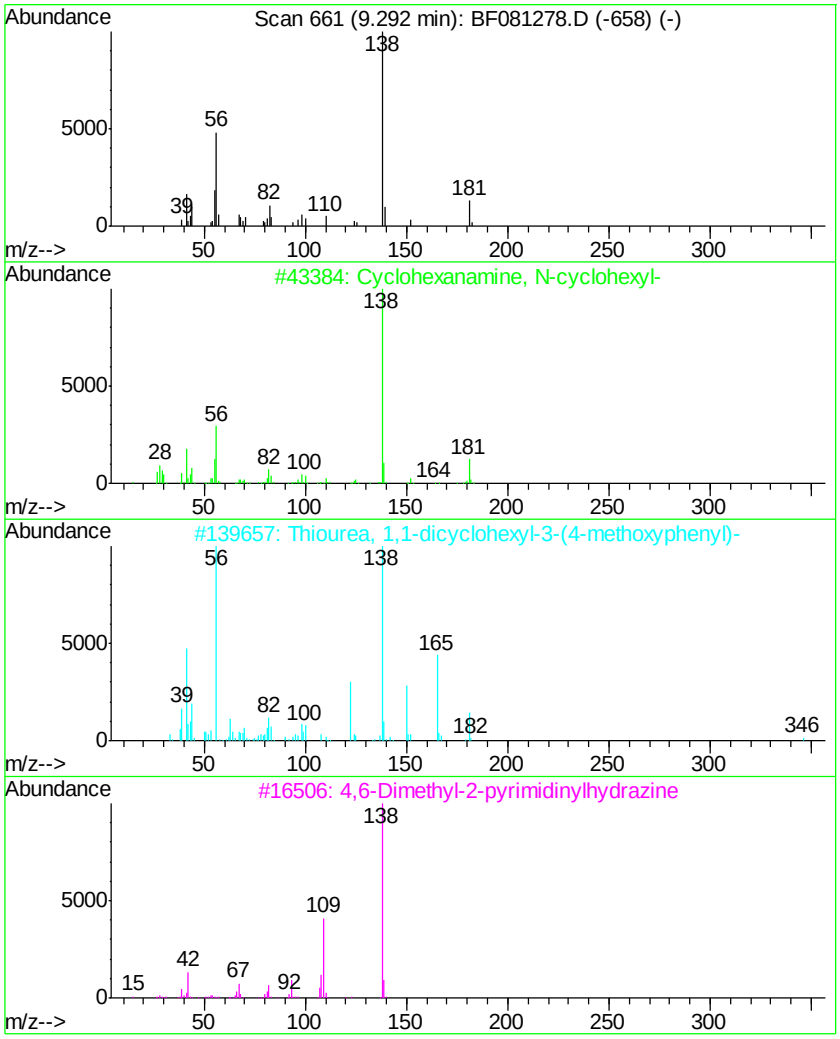
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

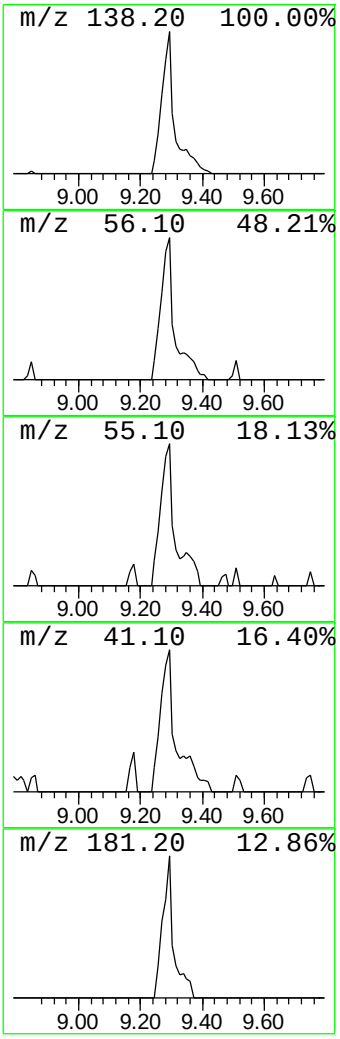
****

Peak Number 5 Cyclohexanamine, N-cyclohexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	5.96 ng	150996	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	93
2	Thiourea, 1,1-dicyclohexyl-3-(4-...	346	C20H30N2OS	351436-82-3	53
3	4,6-Dimethyl-2-pyrimidinylhydrazine	138	C6H10N4	023906-13-0	47
4	N-[1-(Dicyclohexylamino)-2,2,2-t...	416	C19H30F6N2O	1000225-27-8	40
5	3-Amino-4,6-dimethylpyridone-2(1H)	138	C7H10N2O	143708-29-6	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
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Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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
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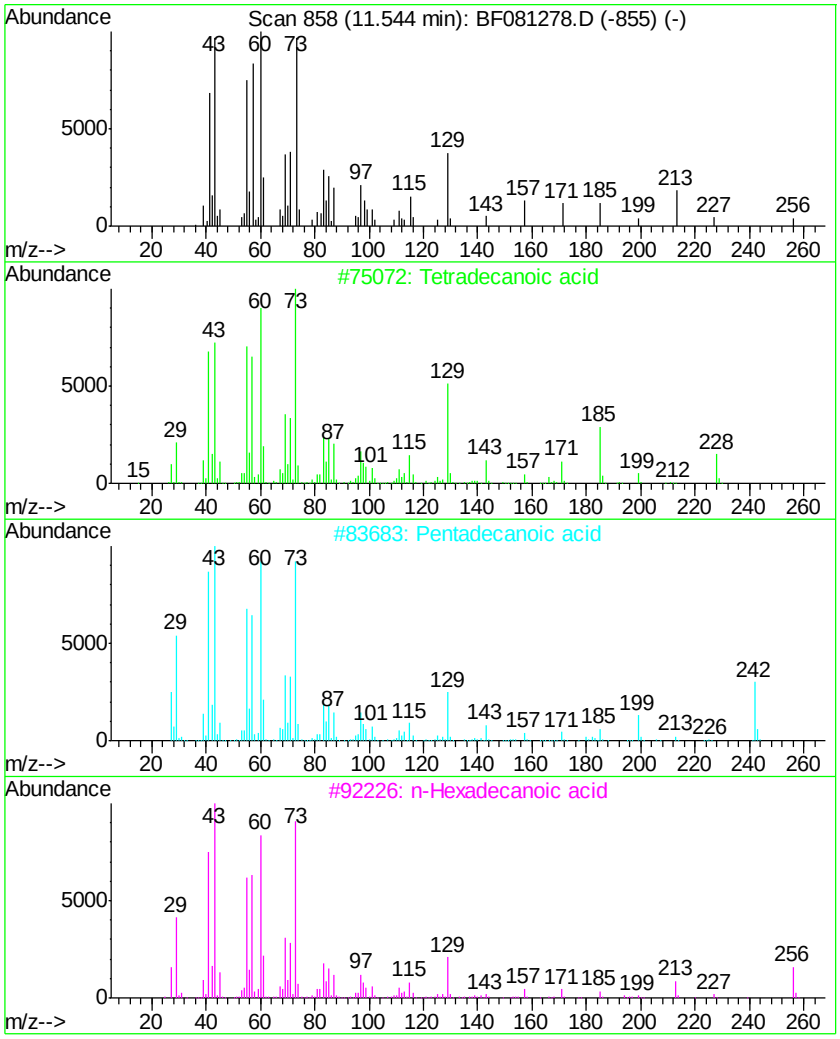
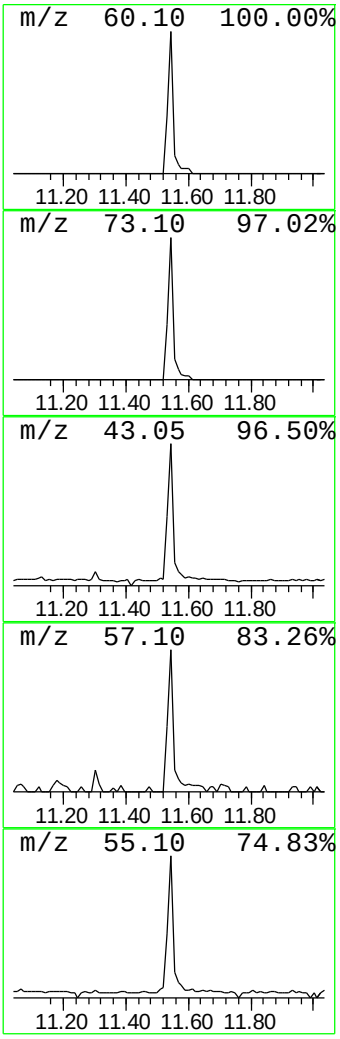
****

Peak Number 6 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	5.17 ng	128904	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Sample : G3467-04
Misc :
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Instrument : BNA_F
ClientSampleId : MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
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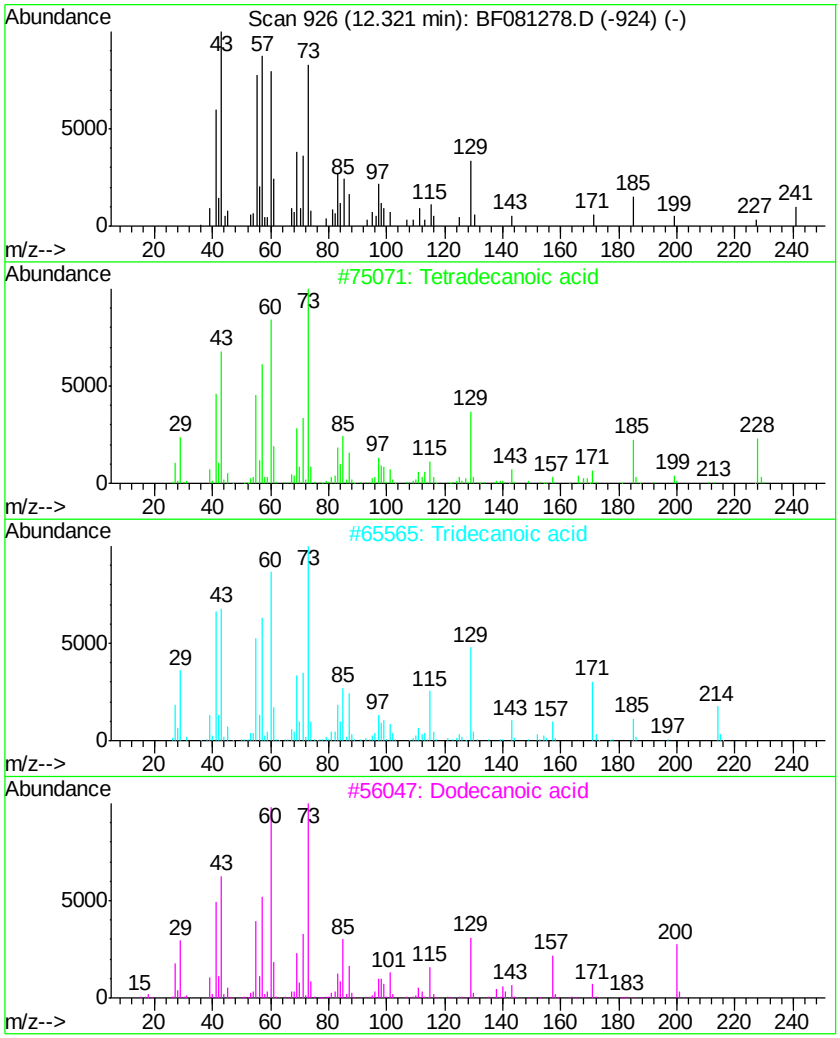
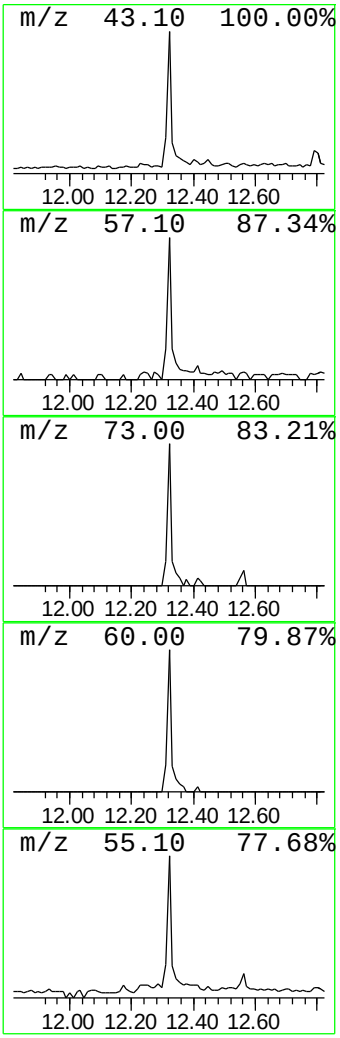
Peak Number 7 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	4.40 ng	102679	Chrysene-d12	13.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	59
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47





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Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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

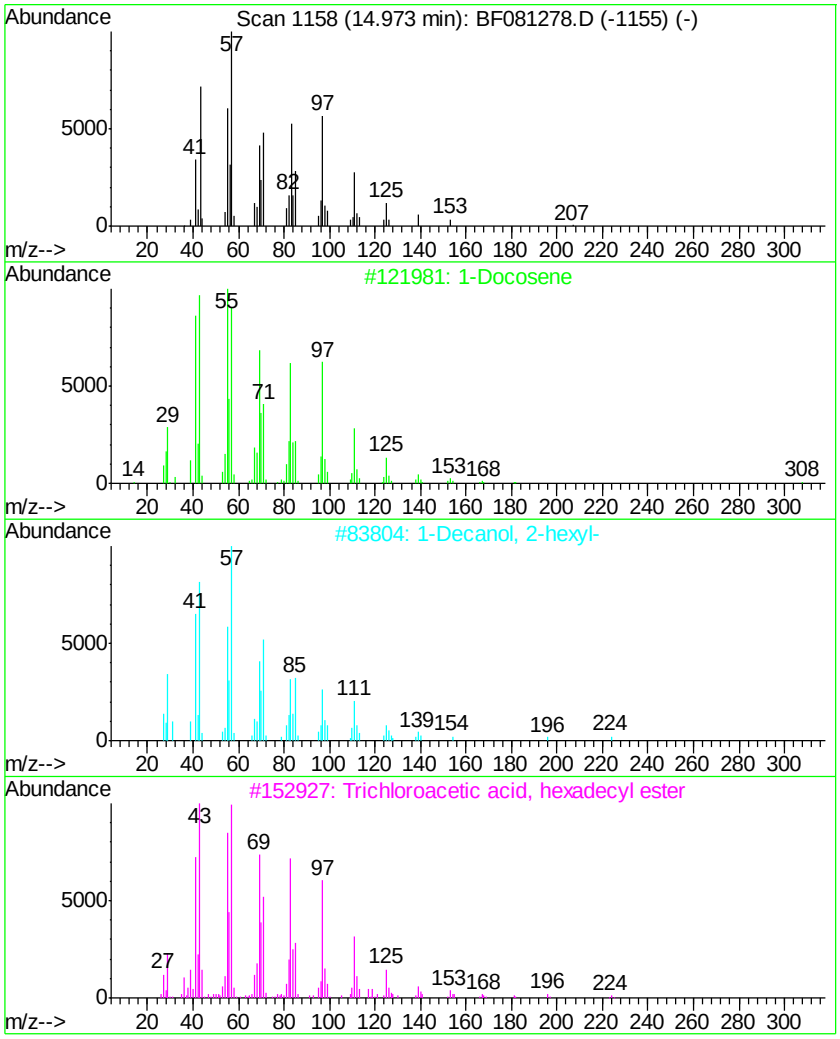
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

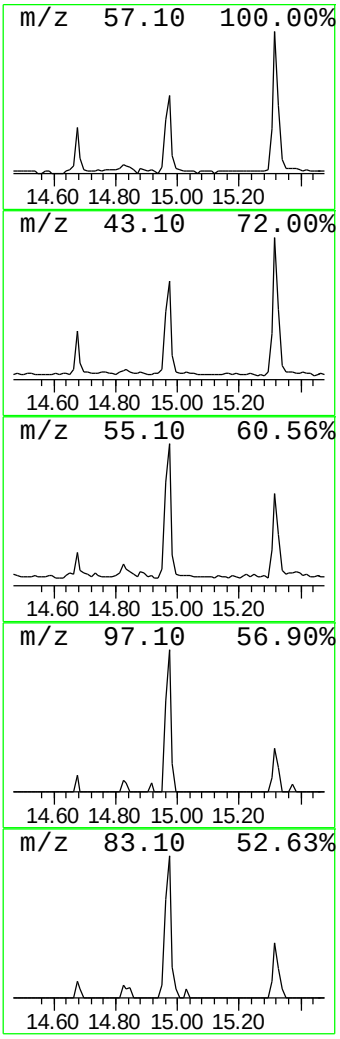
****

Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	5.97 ng	99178	Perylene-d12	14.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	74
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	58
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	52





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Sample : G3467-04
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Instrument : BNA_F
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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
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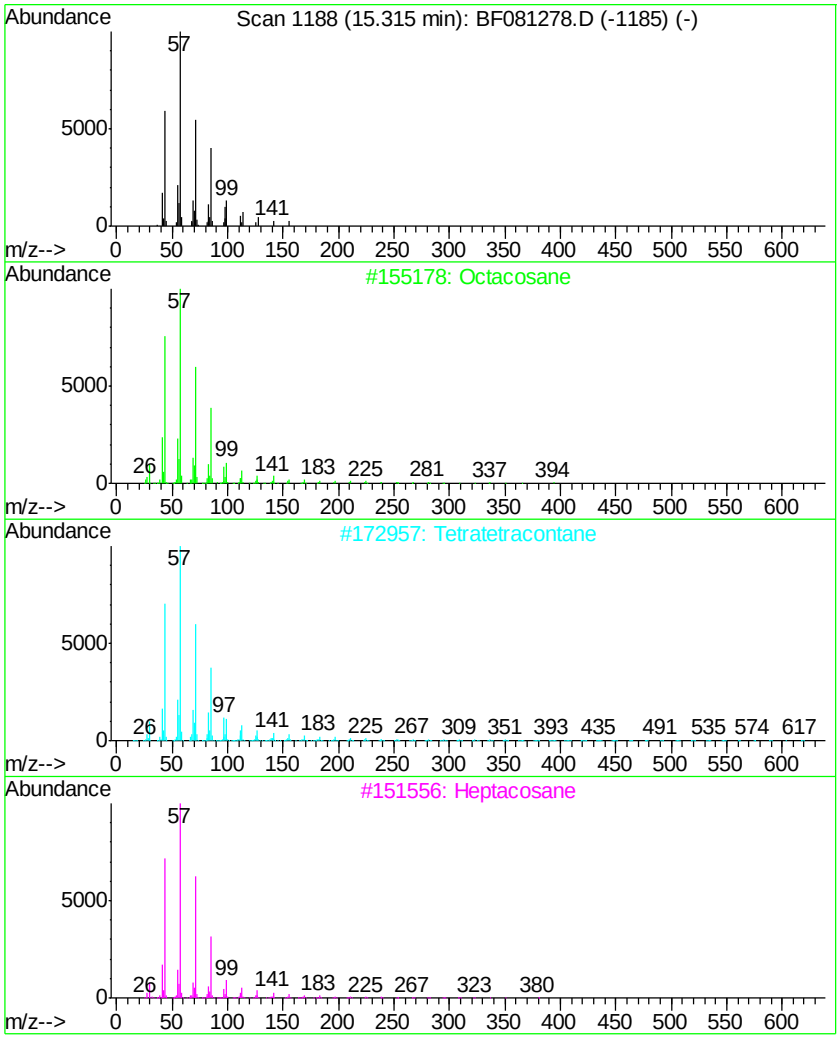
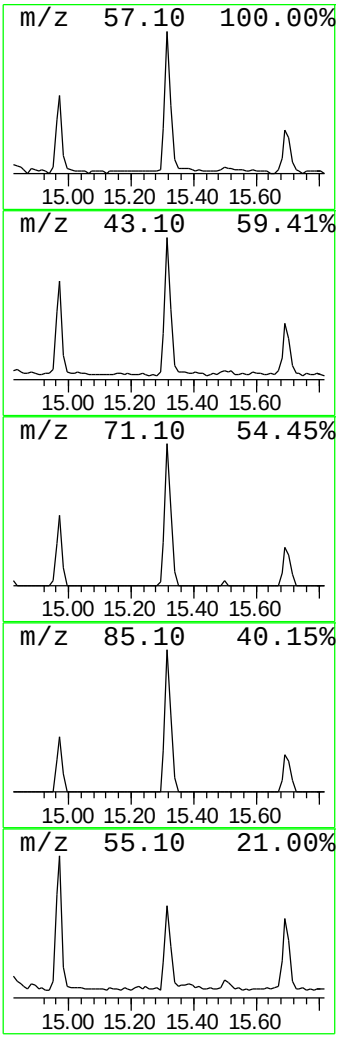
Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	6.07 ng	100922	Perylene-d12	14.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Eicosane	282	C20H42	000112-95-8	87
5	Pentadecane	212	C15H32	000629-62-9	86





Library Search Compound Report

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Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4

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

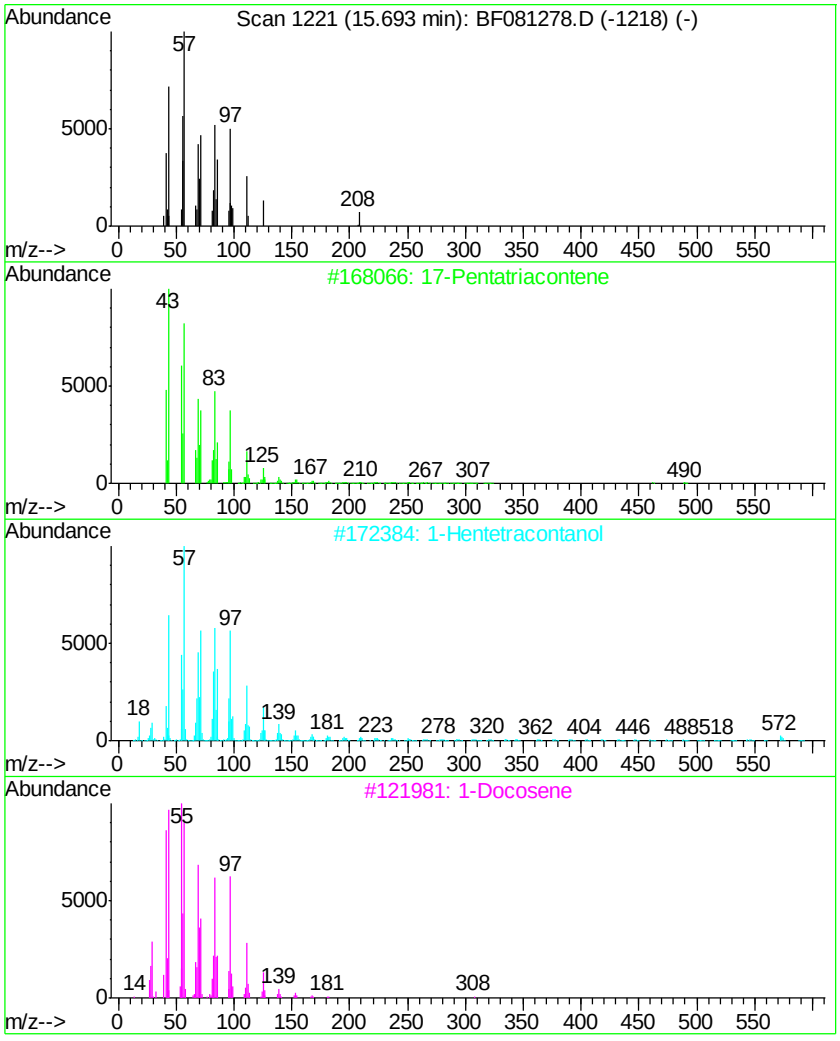
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

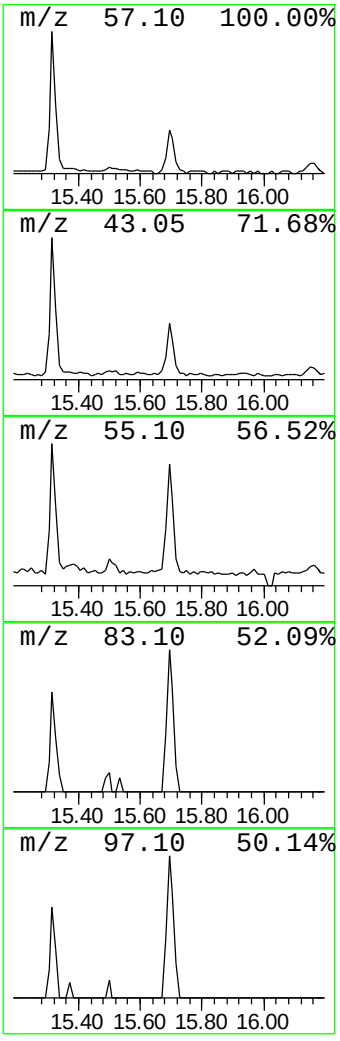
****

Peak Number 10 17-Pentatriacontene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.80 ng	63248	Perylene-d12	14.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	1-Hentetracontanol	593	C41H84O	040710-42-7	78
3	1-Docosene	308	C22H44	001599-67-3	72
4	1-Nonadecene	266	C19H38	018435-45-5	64
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081278.D
Acq On : 29 Aug 2015 18:52
Operator : UM/IZ
Sample : G3467-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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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
2-Pentanone, 4-hy...	4.56	25.2	ng	466796	1	6.48	369904	20.0
unknown6.24	6.24	64.2	ng	1186400	1	6.48	369904	20.0
Ethanol, 2-(2-but...	7.70	12.2	ng	289626	2	7.77	476554	20.0
Cyclohexanamine, ...	9.29	6.0	ng	150996	3	9.51	507078	20.0
Tetradecanoic acid	11.54	5.2	ng	128904	4	10.98	499011	20.0
Tridecanoic acid	12.32	4.4	ng	102679	5	13.59	466336	20.0
1-Docosene	14.97	6.0	ng	99178	6	14.92	332453	20.0
Octacosane	15.32	6.1	ng	100922	6	14.92	332453	20.0
17-Pentatriacontene	15.69	3.8	ng	63248	6	14.92	332453	20.0