LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

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-BF041516.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	2.167	6	7	23	rVB2	111027	416158	5.23%	0.646%
2	5.081	260	262	267	rBV	264177	310227	3.90%	0.481%
3	5.493	295	298	300	rBV	3711810	4573247	57.49%	7.096%
4	6.510	385	387	390	rVB	2768109	2632568	33.10%	4.085%
5	6.659	397	400	402	rBV	5955469	6055141	76.12%	9.396%
6	6.887	418	420	423	rBV	1489637	1894195	23.81%	2.939%
7	7.047	432	434	437	rVB	4956526	5562777	69.93%	8.632%
8	7.459	467	470	472	rVB	4831581	5174456	65.05%	8.029%
9	7.550	475	478	482	rVB3	86146	170497	2.14%	0.265%
10	7.779	494	498	499	rBV2	64325	82265	1.03%	0.128%
11	7.950	510	513	514	rVB2	100879	149568	1.88%	0.232%
12	8.087	522	525	526	rBV	92413	141830	1.78%	0.220%
13	8.133	526	529	530	rVV	180502	299416	3.76%	0.465%
14	8.179	530	533	535	rVV	3007449	2935131	36.90%	4.555%
15	8.213	535	536	539	rVV2	120623	96969	1.22%	0.150%
16	8.259	539	540	542	rVV	84424	111227	1.40%	0.173%
17	8.327	542	546	547	rVV4	131826	283674	3.57%	0.440%
18	8.384	550	551	552	rVV	107244	87347	1.10%	0.136%
19	8.430	554	555	558	rVV2	93711	106645	1.34%	0.165%
20	8.499	558	561	563	rVV	288664	328642	4.13%	0.510%
21	8.556	563	566	570	rVV3	76992	135211	1.70%	0.210%
22	8.636	570	573	576	rVB3	48016	97269	1.22%	0.151%
23	8.704	576	579	580	rBV2	86767	131327	1.65%	0.204%
24	8.727	580	581	582	rVV	207274	166862	2.10%	0.259%
25	8.807	586	588	590	rVB2	111858	155309	1.95%	0.241%
26	8.876	590	594	596	rBV2	124606	310385	3.90%	0.482%
27	8.945	598	600	603	rVB2	122365	182335	2.29%	0.283%
28	9.025	605	607	609	rVB2	104946	127530	1.60%	0.198%
29	9.093	612	613	615	rBV2	72871	114528	1.44%	0.178%
30	9.253	624	627	630	rBV	5358945	7954442	100.00%	12.343%
31	9.345	630	635	639	rVB6	62149	161219	2.03%	0.250%
32	9.539	648	652	655	rVB4	62418	174354	2.19%	0.271%
33	9.653	660	662	664	rVV	276379	333149	4.19%	0.517%
34	9.756	666	671	672	rBV5	33437	85359	1.07%	0.132%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

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-BF041516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.870	680	681	684	rBV	113236	89863	1.13%	0.139%
36	9.927	684	686	695	rVB2	1974834	3198365	40.21%	4.963%
37	10.350	721	723	726	rVB2	203642	312791	3.93%	0.485%
38	10.442	729	731	733	rBV	130380	114017	1.43%	0.177%
39	10.716	752	755	758	rBV2	3382175	4271778	53.70%	6.629%
40	10.808	761	763	765	rVV3	44911	108859	1.37%	0.169%
41	10.842	765	766	771	rVB	208066	231180	2.91%	0.359%
42	11.288	803	805	807	rBV	163008	149594	1.88%	0.232%
43	11.413	814	816	819	rVB	2866411	2504114	31.48%	3.886%
44	11.470	819	821	825	rBV2	67801	101958	1.28%	0.158%
45	11.951	861	863	865	rBV	225704	303246	3.81%	0.471%
46	12.076	871	874	876	rBV	634093	803896	10.11%	1.247%
47	12.728	930	931	937	rBV	139637	283048	3.56%	0.439%
48	12.831	937	940	942	rVV	147006	204322	2.57%	0.317%
49	13.002	952	955	958	rBV	4957896	5653059	71.07%	8.772%
50	13.208	971	973	975	rBV2	96624	110839	1.39%	0.172%
51	13.894	1031	1033	1038	rBV2	74393	131523	1.65%	0.204%
52	14.042	1044	1046	1049	rBV2	1611151	1867449	23.48%	2.898%
53	15.414	1163	1166	1169	rBV	858081	1067106	13.42%	1.656%
54	15.482	1169	1172	1175	rVB	1137393	1395882	17.55%	2.166%

Sum of corrected areas: 64444148

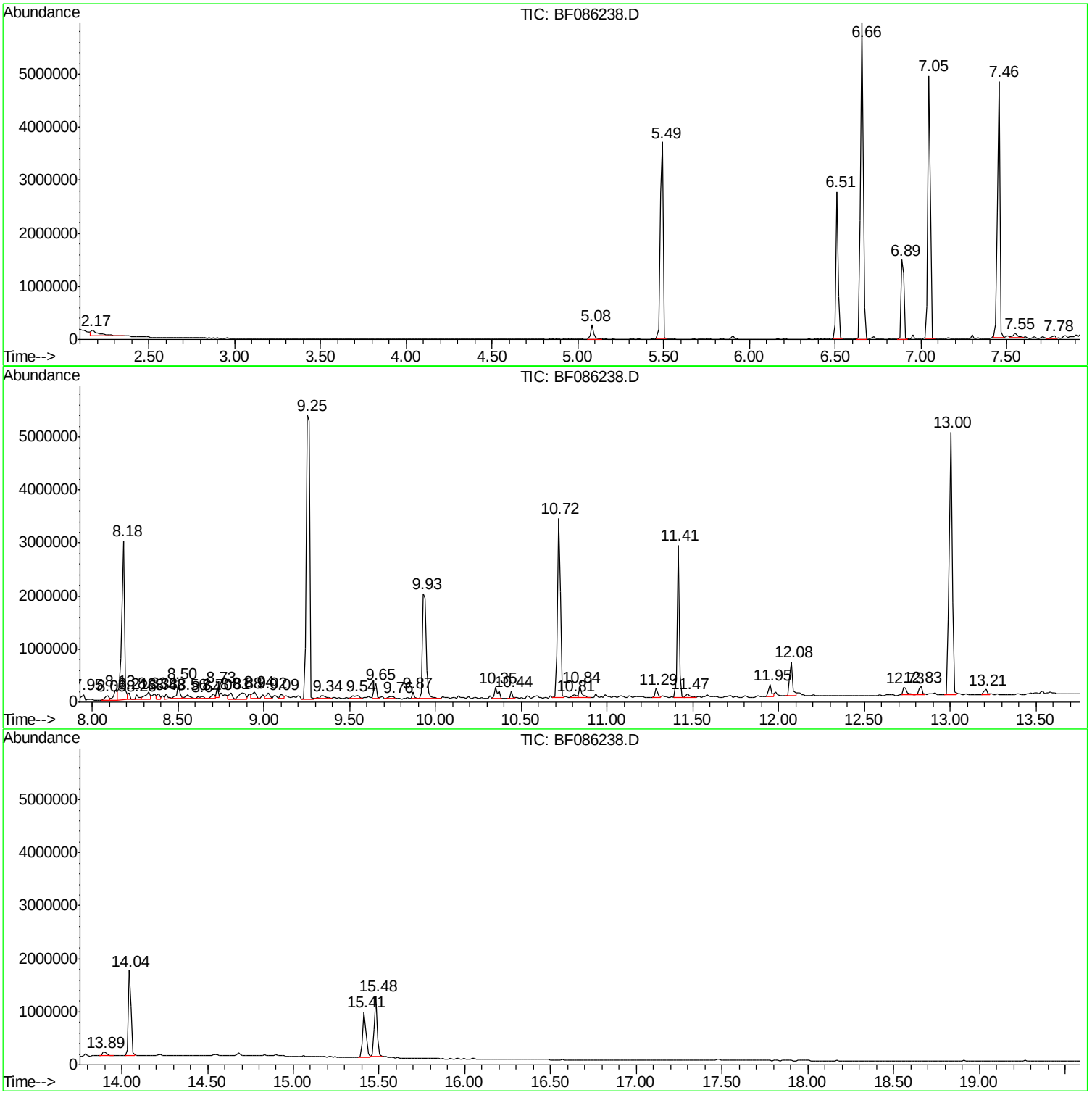
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

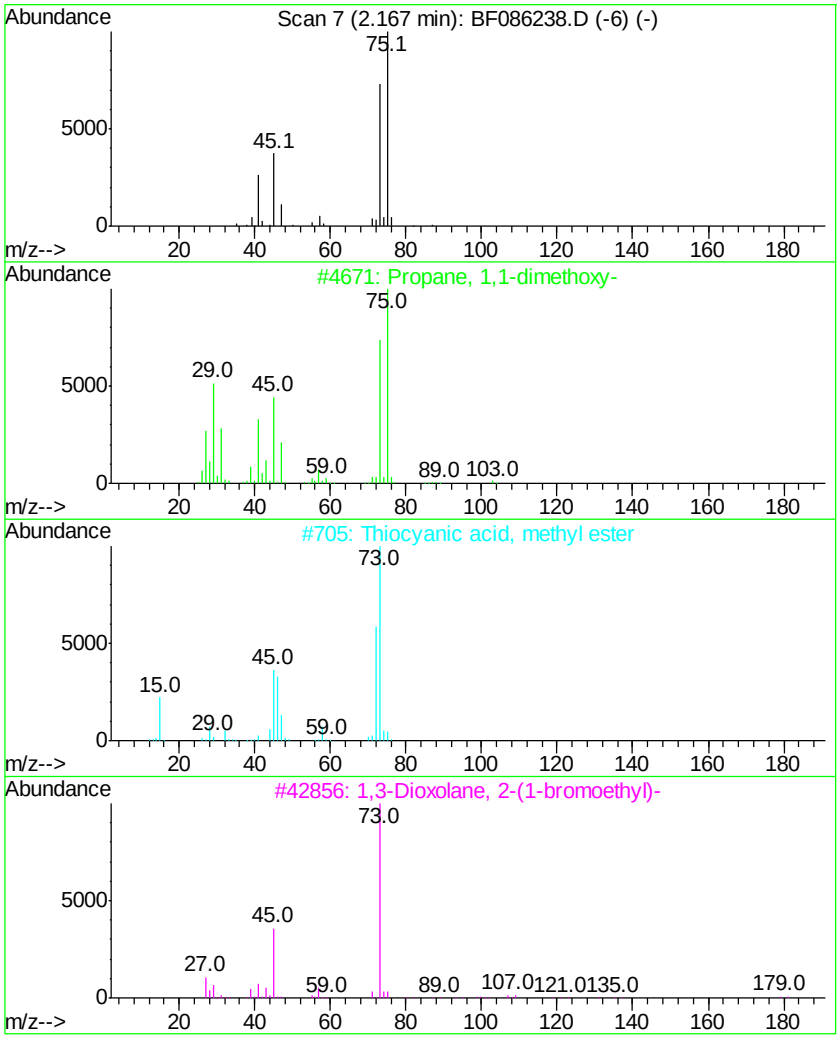
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

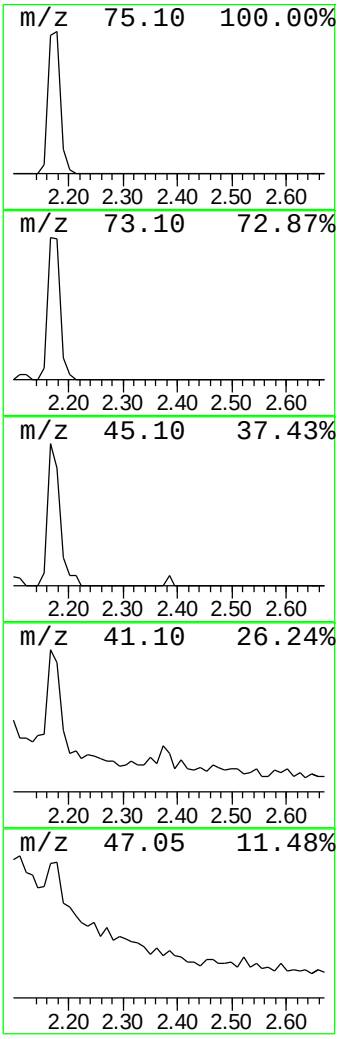
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	4.39 ng	416158	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	12
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

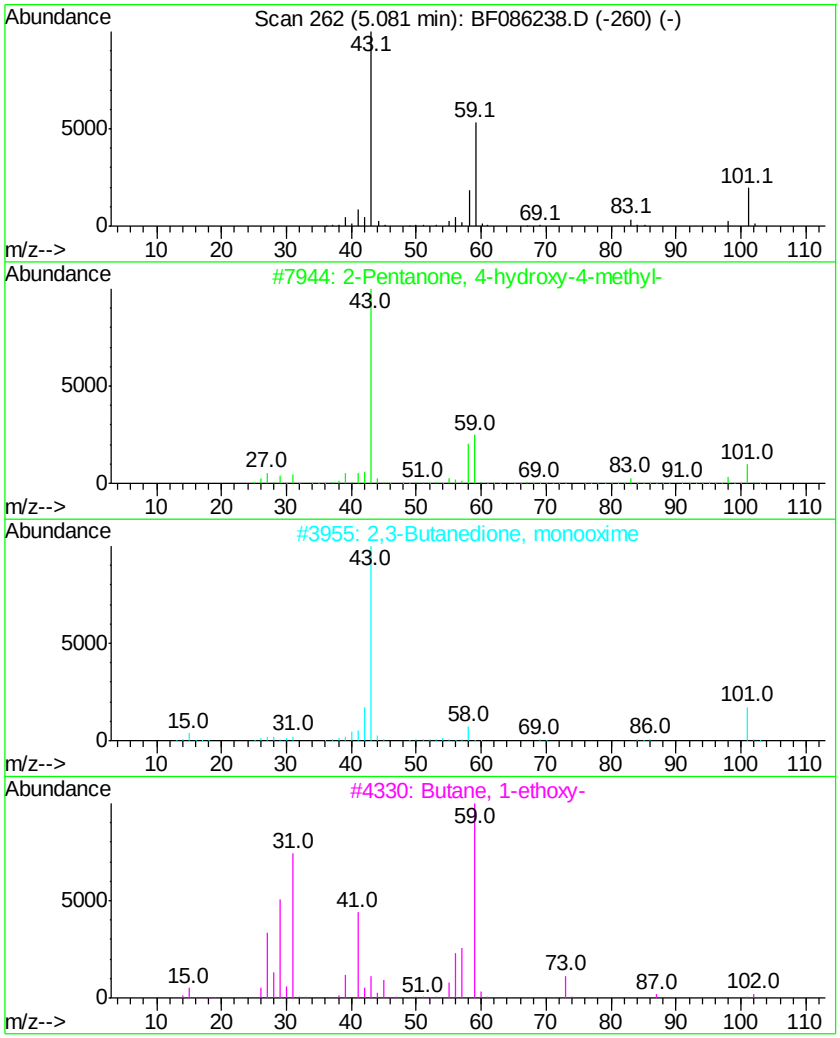
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

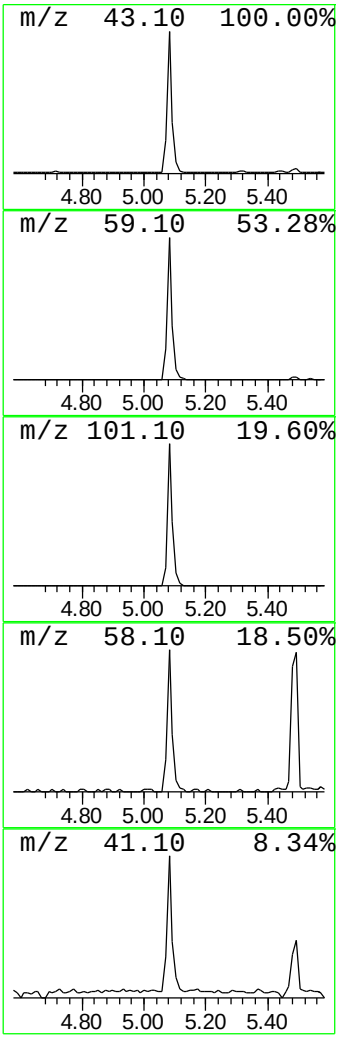
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	3.28 ng	310227	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
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Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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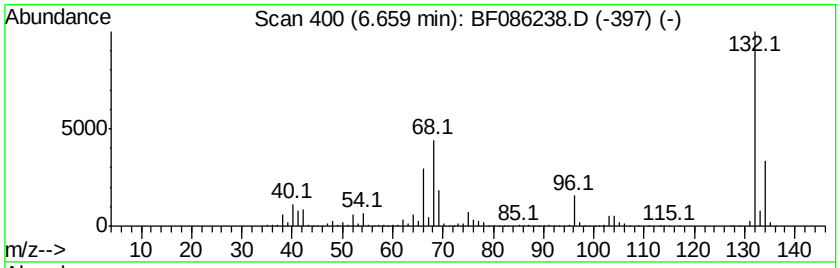
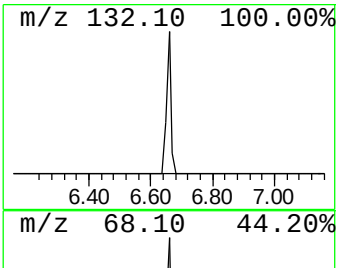
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	63.93 ng	6055140	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

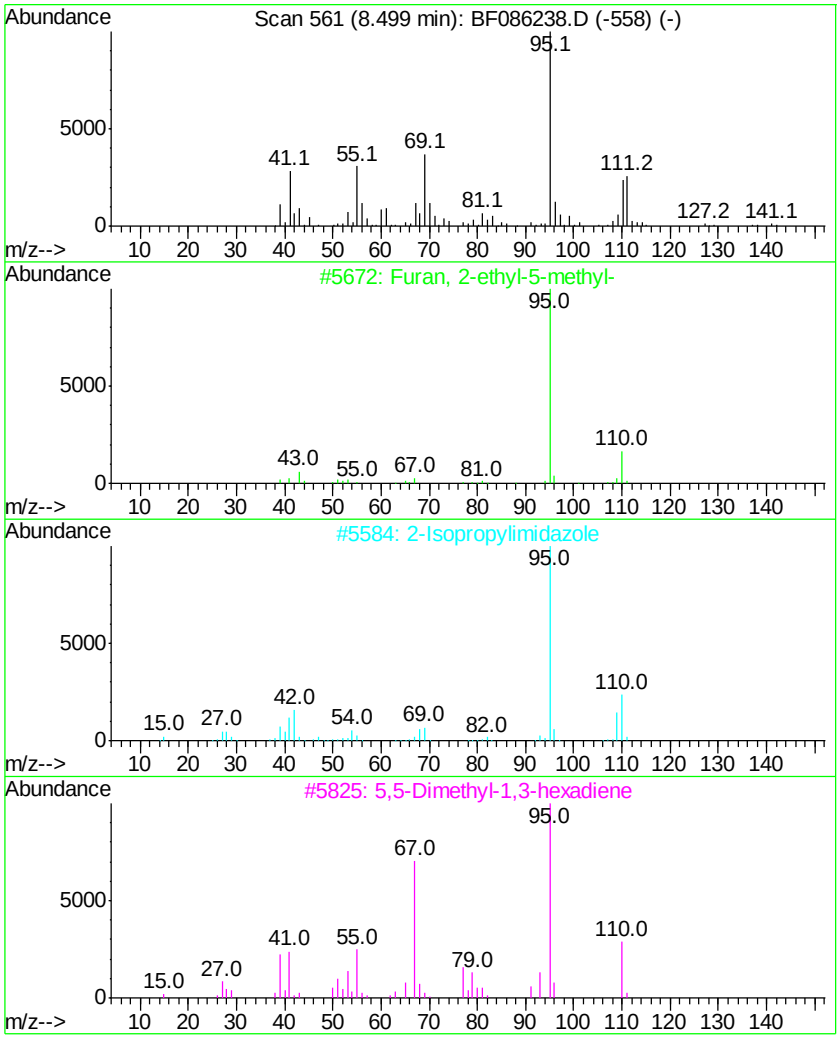
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

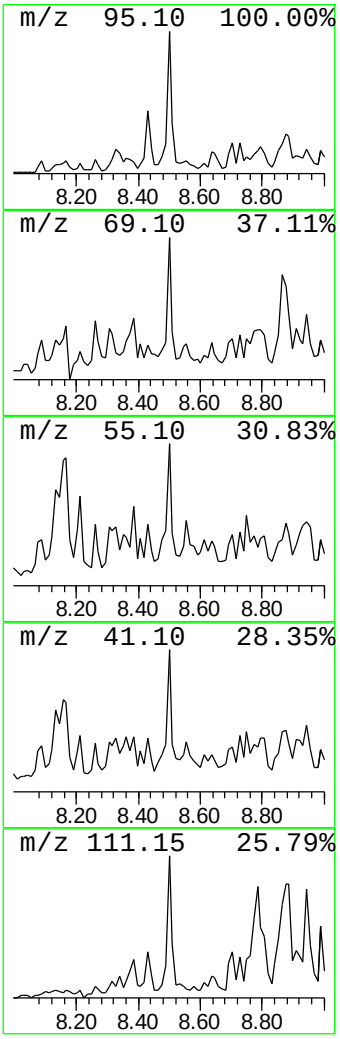
****

Peak Number 5 Furan, 2-ethyl-5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	2.24 ng	328642	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	53
2	2-Isopropylimidazole	110	C6H10N2	036947-68-9	53
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	53
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	53
5	2-Furanecarboxylic acid, 3,5-dim...	222	C13H18O3	1000278-87-2	42





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Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
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Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

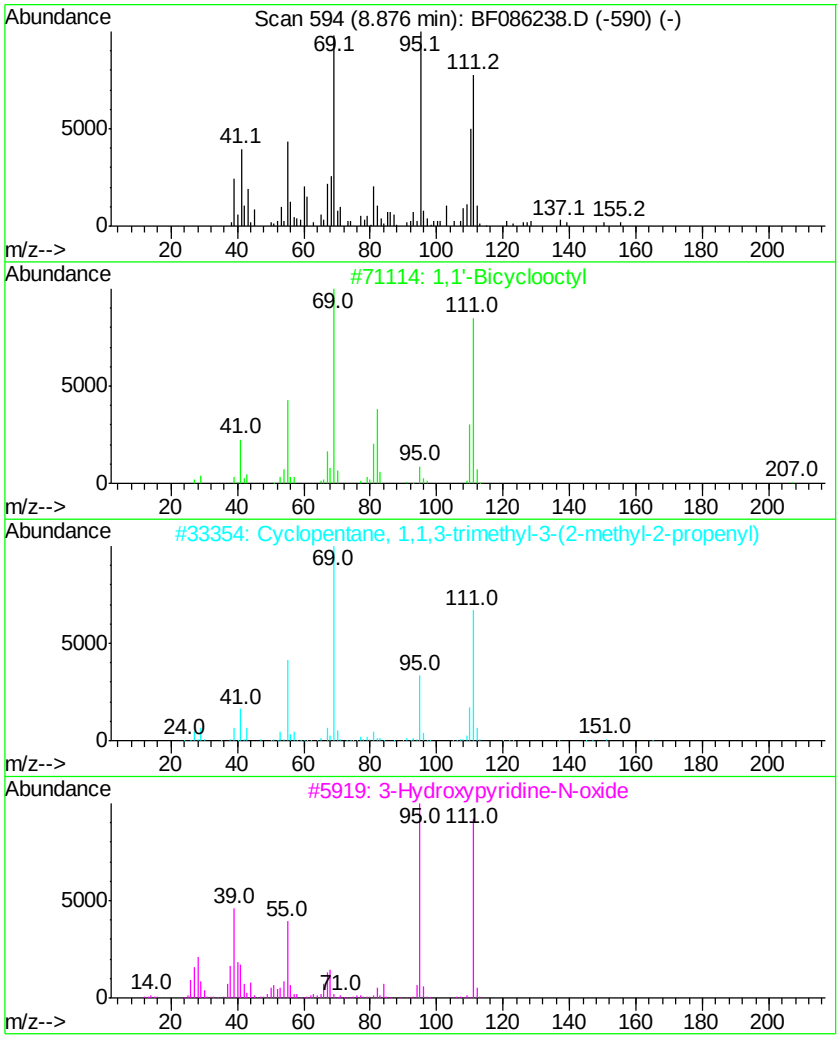
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

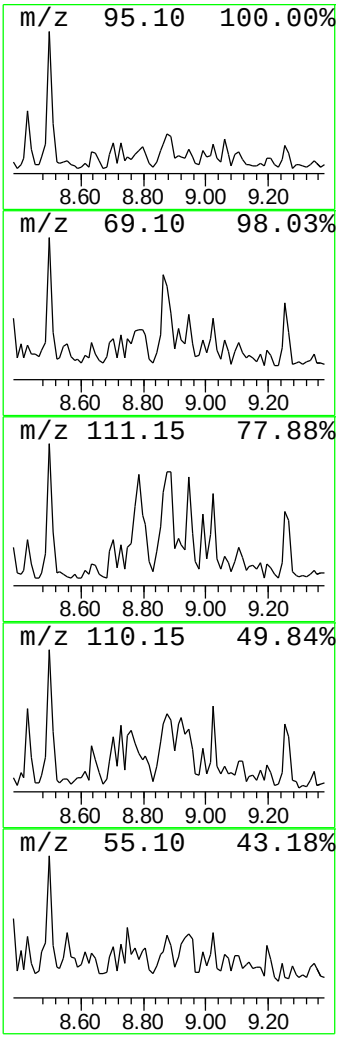
****

Peak Number 6 unknown8.88 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	2.11 ng	310385	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	47
2	Cyclopentane, 1,1,3-trimethyl-3-...	166	C12H22	074421-09-3	43
3	3-Hydroxypyridine-N-oxide	111	C5H5NO2	006602-28-4	38
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	38
5	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	38





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Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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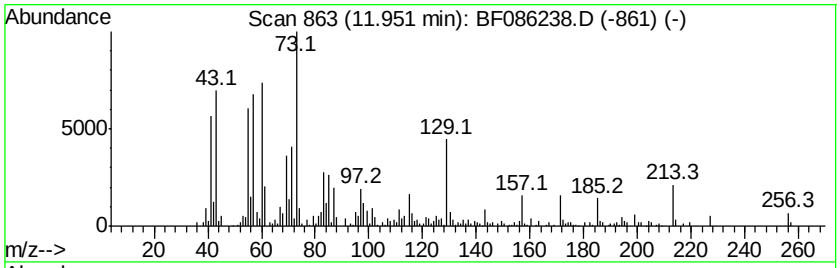
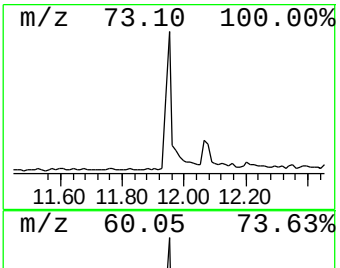
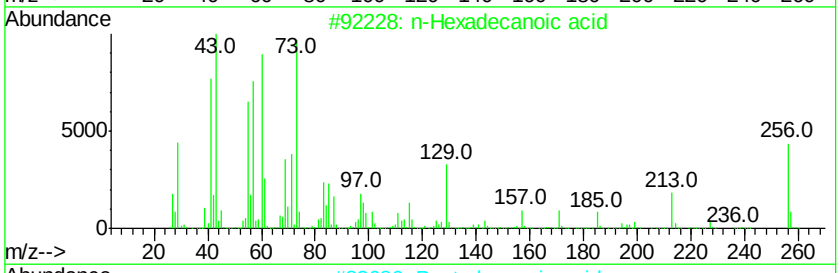
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

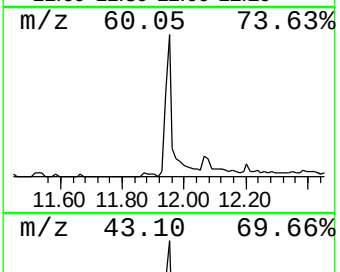
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.42 ng	303246	Phenanthrene-d10	11.41

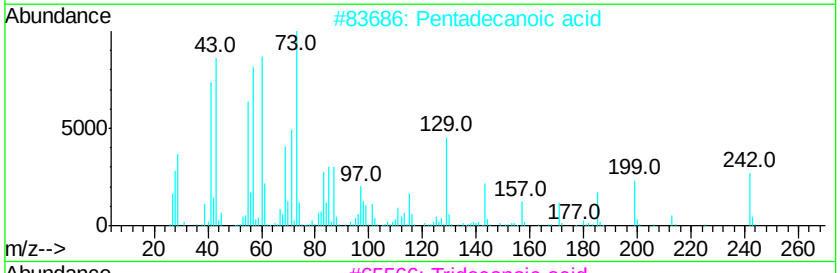
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18

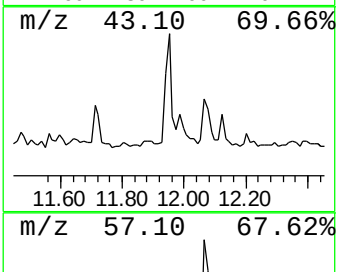


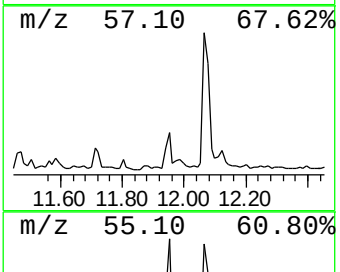


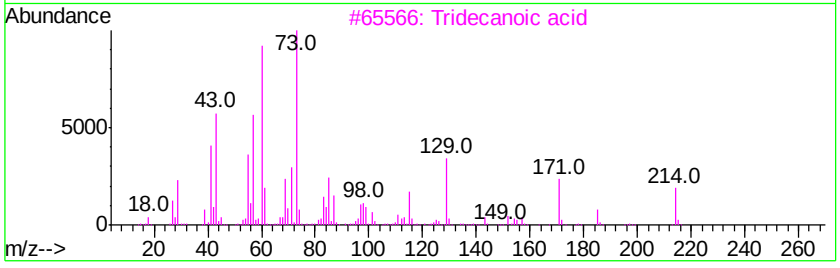


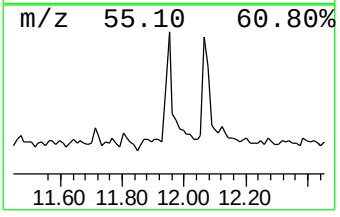












Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

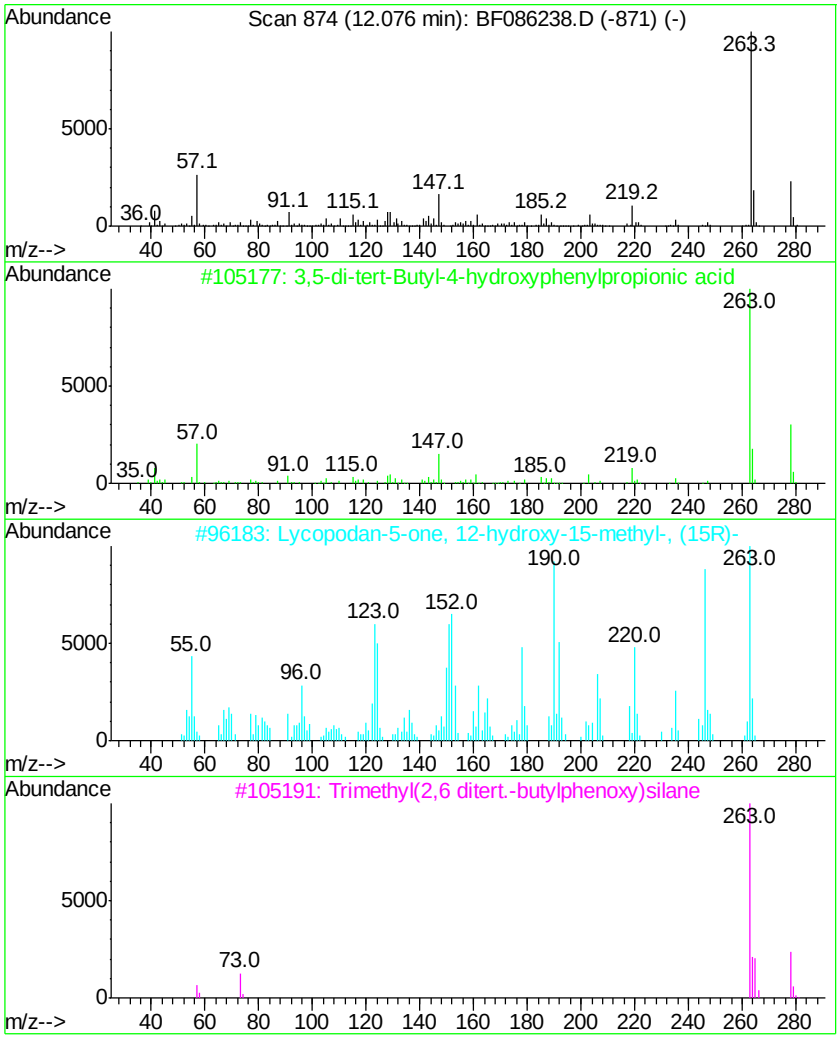
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

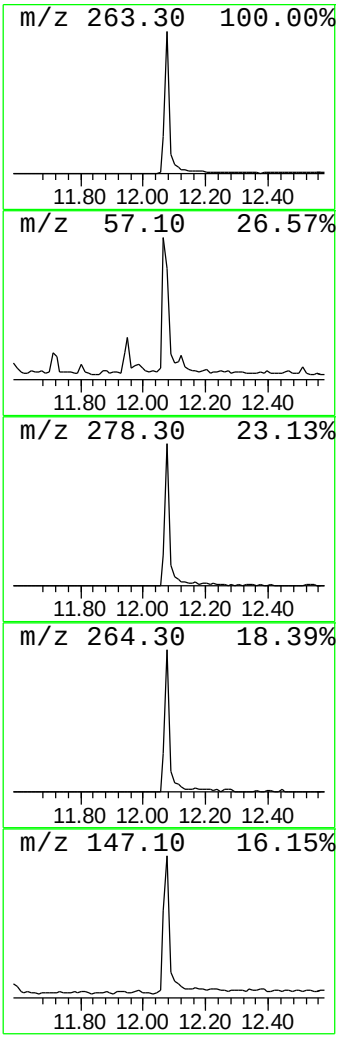
****

Peak Number 8 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	6.42 ng	803896	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	94
2	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	006900-92-1	92
3	Trimethyl(2,6 ditert.-butylpheno...	278	C17H30OSi	010416-73-6	59
4	Pentan-2-one, 4-(2-fluorenylimino)-	263	C18H17NO	050651-58-6	53
5	6-Oxo-5-phenyl-2,3,5,6-tetrahydr...	263	C16H13N3O	087365-22-8	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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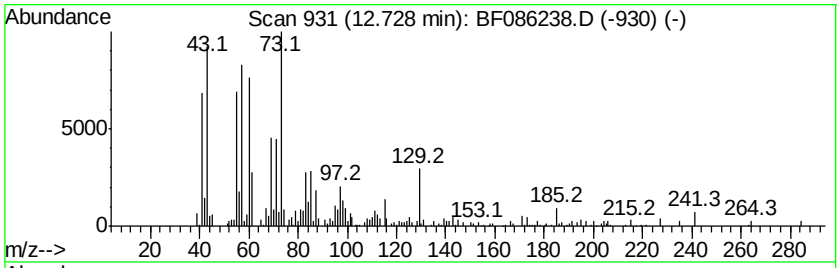
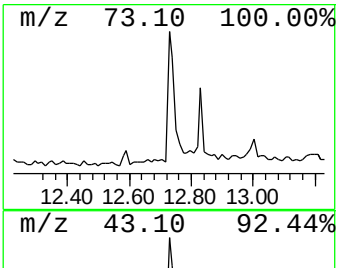
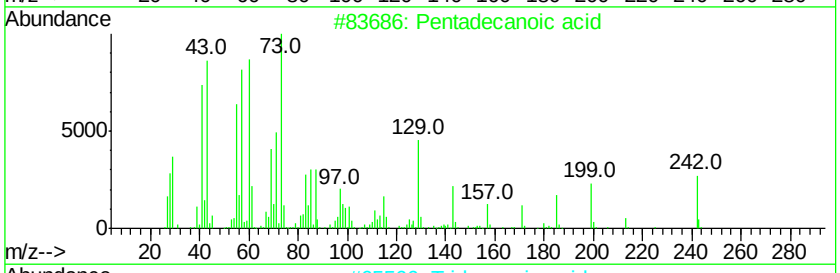
Peak Number 9 Pentadecanoic acid Concentration Rank 8

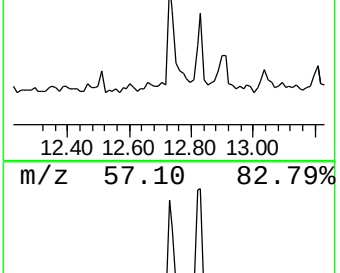
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.26 ng	283048	Phenanthrene-d10	11.41

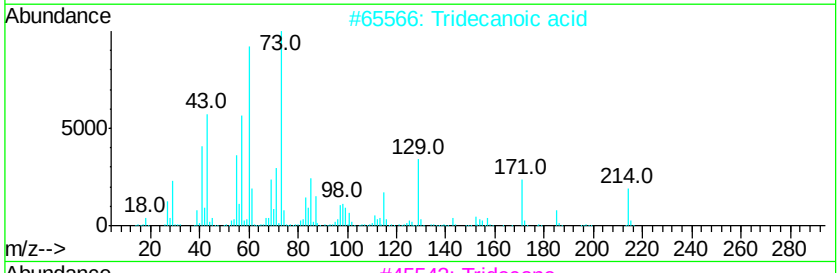
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Tridecane	184	C13H28	000629-50-5	18
4	l-Tyrosinol	167	C9H13NO2	1000131-27-0	18
5	Dodecane	170	C12H26	000112-40-3	18

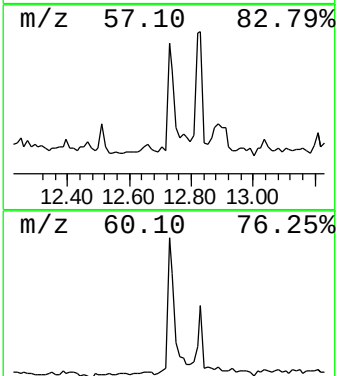


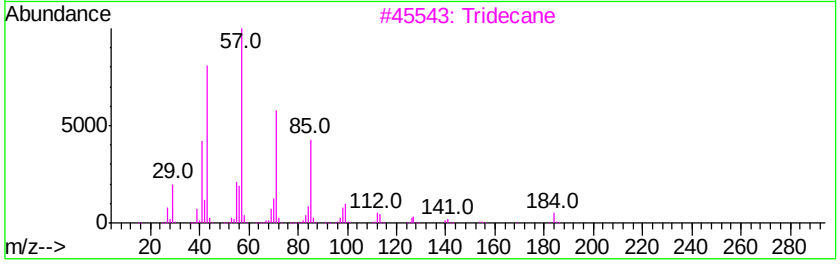


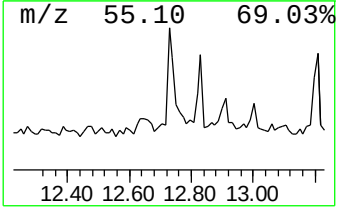












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Data File : BF086238.D
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Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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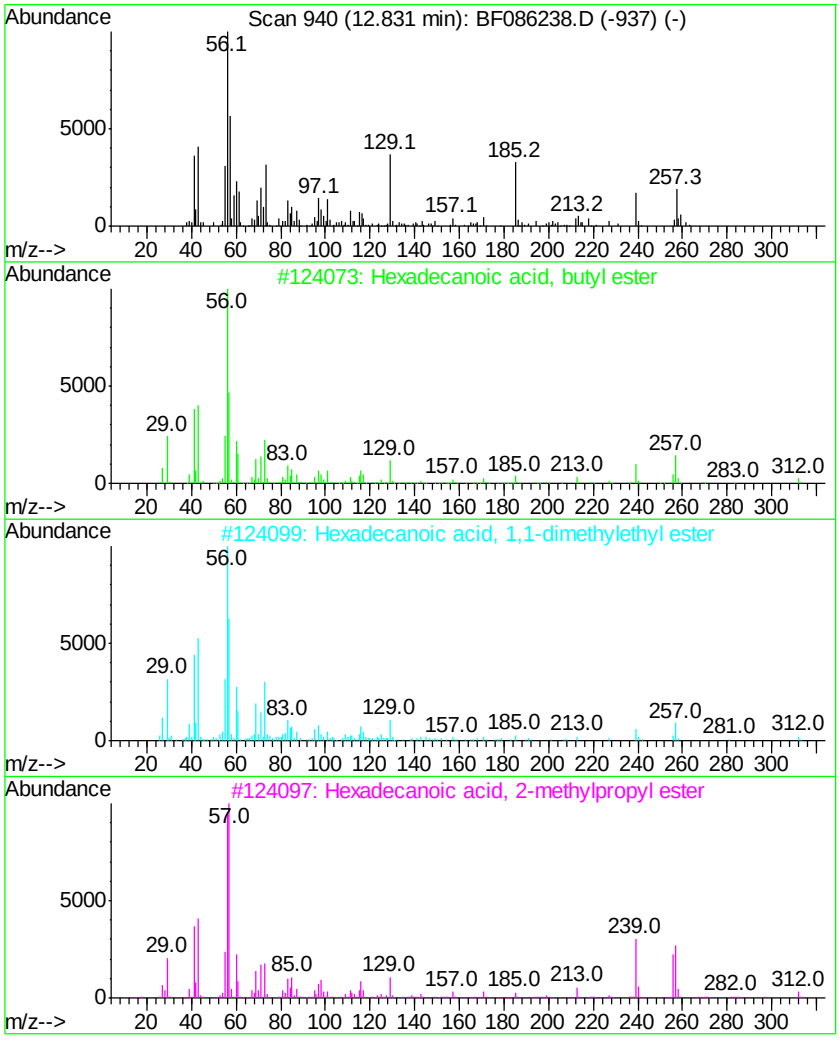
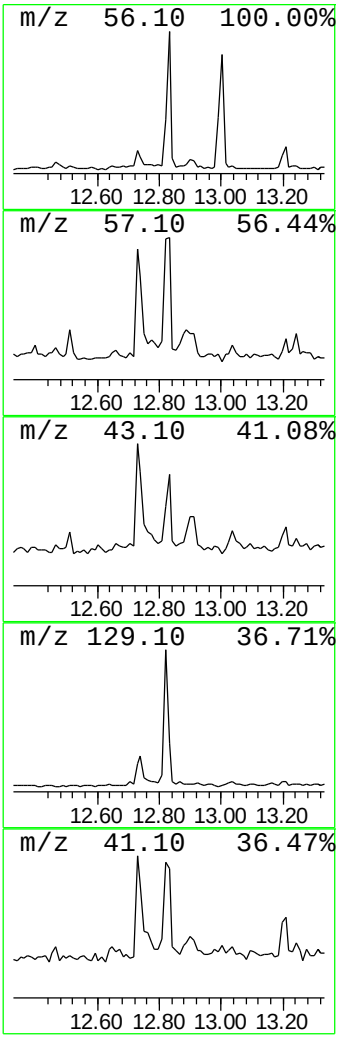
Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.19 ng	204322	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	47
4	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	25
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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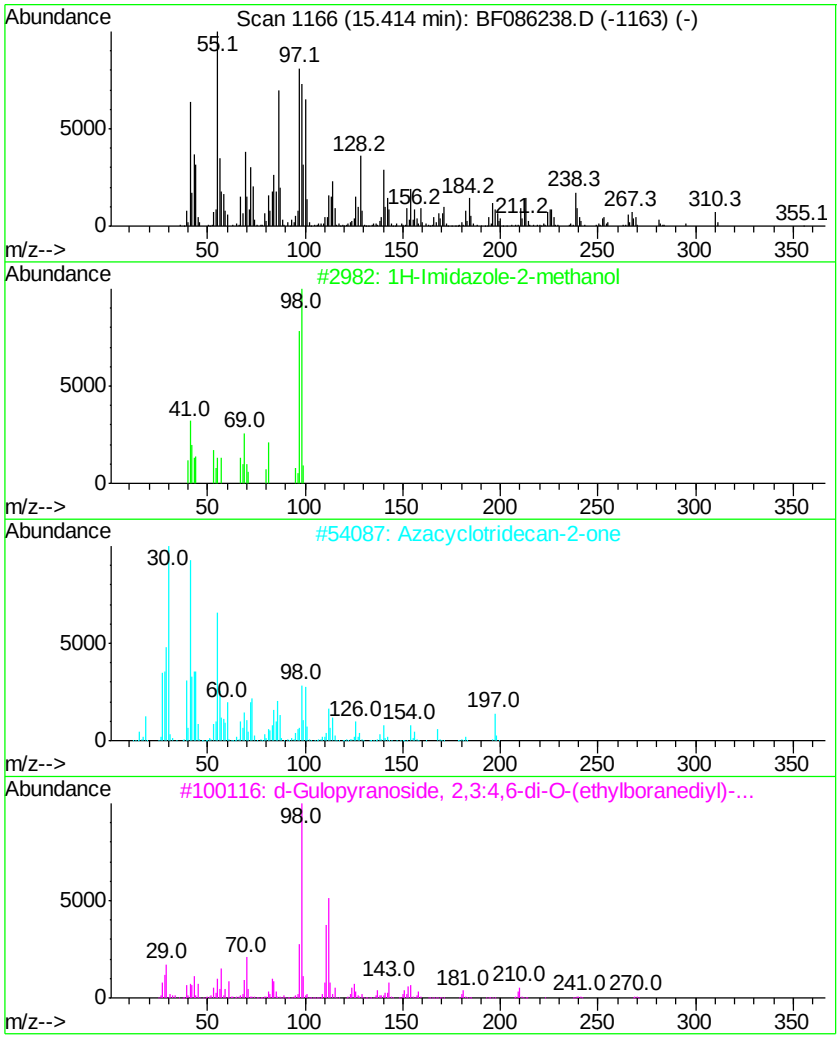
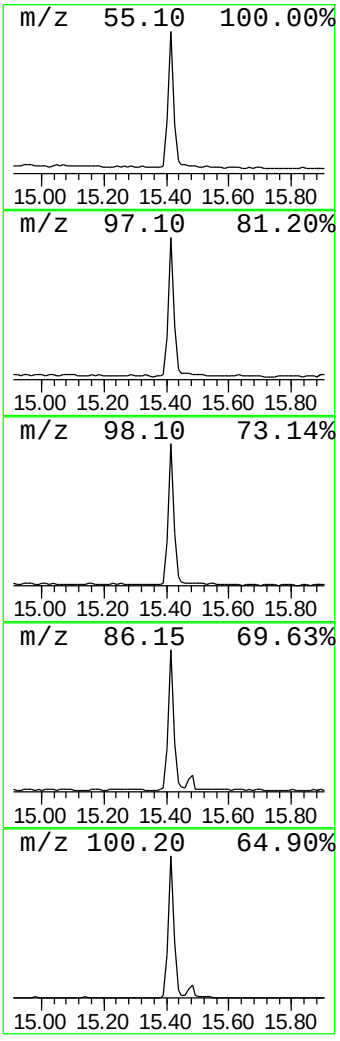
Peak Number 11 unknown15.41 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	15.29 ng	1067110	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole-2-methanol	98	C4H6N2O	003724-26-3	25
2	Azacyclotridecan-2-one	197	C12H23NO	000947-04-6	25
3	d-Gulopyranoside, 2,3:4,6-di-O-(...	270	C11H20B2O6	1000149-94-5	18
4	trans-2-Oxabicyclo[4.4.0]decane	140	C9H16O	059958-46-2	18
5	1,5-Di(1-piperidinyl)pentane	238	C15H30N2	024362-44-5	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
Data File : BF086238.D
Acq On : 16 Apr 2016 2:19
Operator : UM/SJ
Sample : H2402-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2-4-7-16

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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
Propane, 1,1-dime...	2.17	4.4	ng	416158	1	6.90	1894200	20.0
2-Pentanone, 4-hy...	5.08	3.3	ng	310227	1	6.90	1894200	20.0
unknown6.66	6.66	63.9	ng	6055140	1	6.90	1894200	20.0
Furan, 2-ethyl-5-...	8.50	2.2	ng	328642	2	8.18	2935130	20.0
unknown8.88	8.88	2.1	ng	310385	2	8.18	2935130	20.0
n-Hexadecanoic acid	11.95	2.4	ng	303246	4	11.41	2504110	20.0
3,5-di-tert-Butyl...	12.08	6.4	ng	803896	4	11.41	2504110	20.0
Pentadecanoic acid	12.73	2.3	ng	283048	4	11.41	2504110	20.0
Hexadecanoic acid...	12.83	2.2	ng	204322	5	14.04	1867450	20.0
unknown15.41	15.41	15.3	ng	1067110	6	15.48	1395880	20.0