LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087046.D
Acq On : 15 May 2016 3:56
Operator : UM/SJ
Sample : H3052-01
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

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-BF050916.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	1.736	12	13	55	rVB	3474468	6985344	100.00%	16.917%
2	4.079	215	218	231	rVB	90377	165417	2.37%	0.401%
3	4.730	274	275	289	rBV	182833	355733	5.09%	0.861%
4	5.199	314	316	333	rBV	1702630	1944664	27.84%	4.709%
5	6.273	408	410	417	rBV	1100020	1384976	19.83%	3.354%
6	6.387	417	420	422	rBV	2903030	3537842	50.65%	8.568%
7	6.605	437	439	445	rVB	789046	963535	13.79%	2.333%
8	6.765	450	453	456	rBV	3246692	2939827	42.09%	7.119%
9	7.187	487	490	492	rBV	2972265	3126128	44.75%	7.571%
10	7.896	550	552	555	rBV	1369052	1242991	17.79%	3.010%
11	8.205	577	579	584	rBV	62905	82075	1.17%	0.199%
12	8.833	632	634	638	rVB	49194	76551	1.10%	0.185%
13	8.982	644	647	649	rBV	4676365	4962090	71.04%	12.017%
14	9.382	680	682	684	rBV	150356	136810	1.96%	0.331%
15	9.645	702	705	708	rBV	1489331	1357437	19.43%	3.287%
16	10.091	739	744	745	rBV2	97986	106860	1.53%	0.259%
17	10.434	771	774	777	rBV	2577371	2638124	37.77%	6.389%
18	10.559	783	785	791	rVB	110812	127063	1.82%	0.308%
19	10.822	806	808	809	rBV	50253	73163	1.05%	0.177%
20	11.119	832	834	837	rBV	1216304	1227447	17.57%	2.973%
21	11.622	873	878	880	rBV	85459	162940	2.33%	0.395%
22	11.679	880	883	893	rVB	981167	1106626	15.84%	2.680%
23	12.377	940	944	947	rBV	149115	227796	3.26%	0.552%
24	12.457	949	951	957	rVV	210955	325618	4.66%	0.789%
25	12.708	970	973	976	rBV	3703738	3959452	56.68%	9.589%
26	13.062	1001	1004	1006	rVB	80579	129249	1.85%	0.313%
27	13.622	1051	1053	1057	rBV	94453	124318	1.78%	0.301%
28	13.748	1061	1064	1067	rBV	1001409	964730	13.81%	2.336%
29	15.108	1180	1183	1189	rBV	718884	858083	12.28%	2.078%

Sum of corrected areas: 41292889

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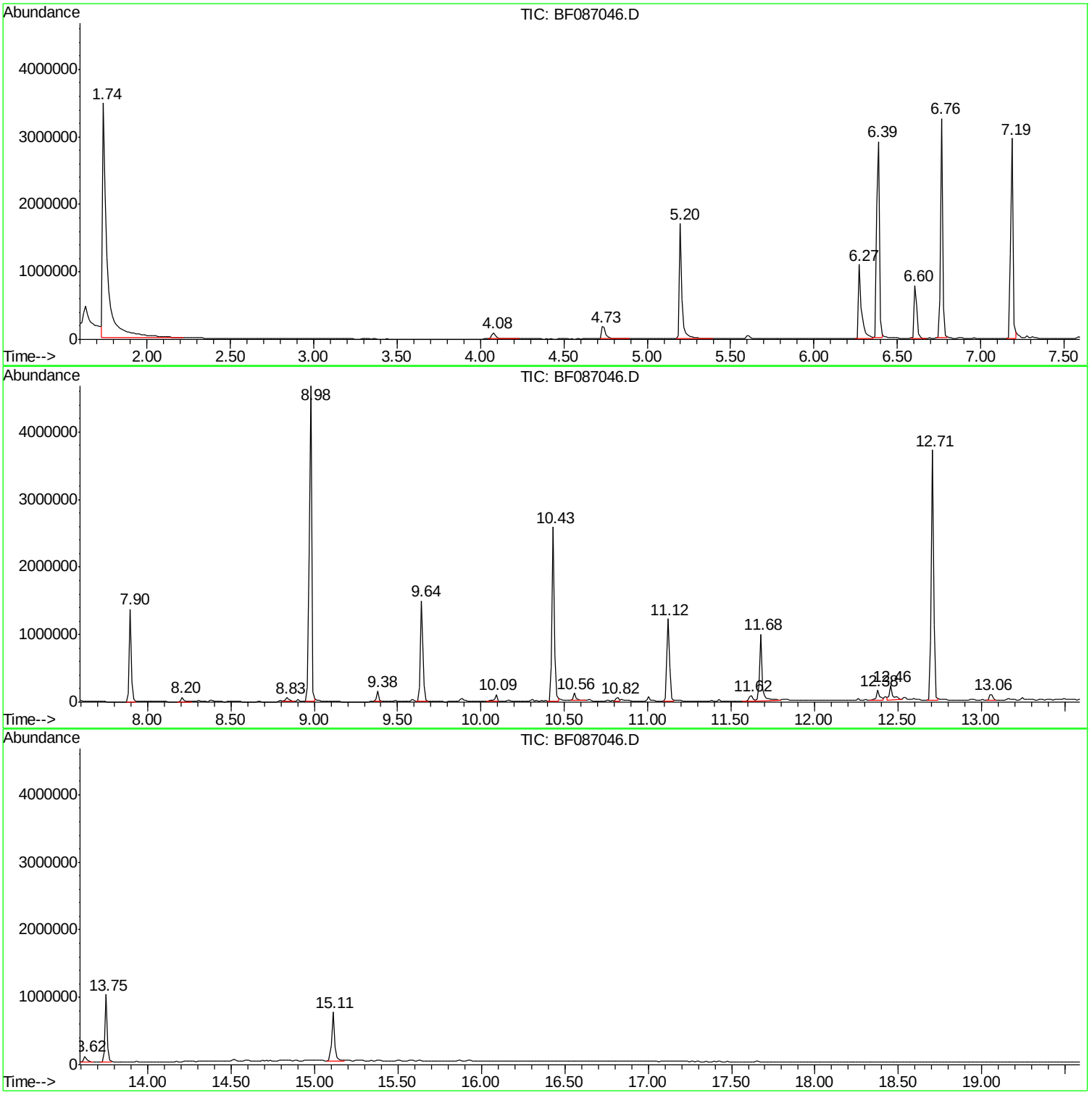
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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TIC Library : C:\DATABASE\NIST02.L
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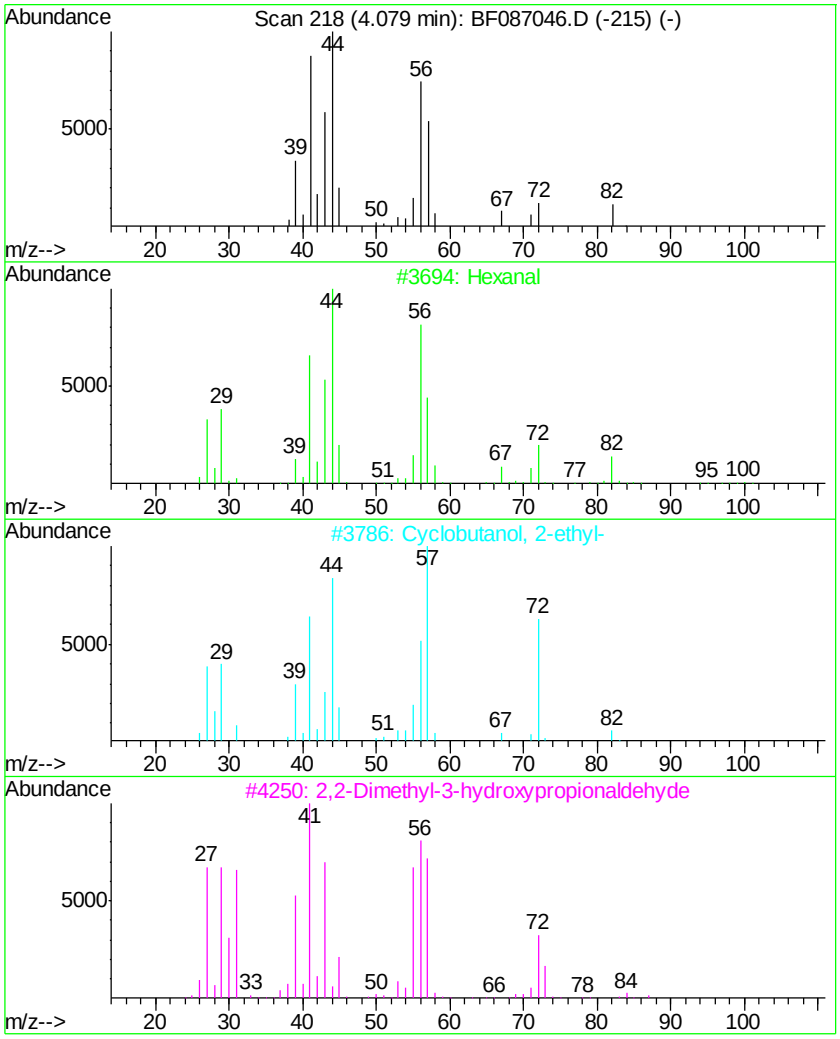
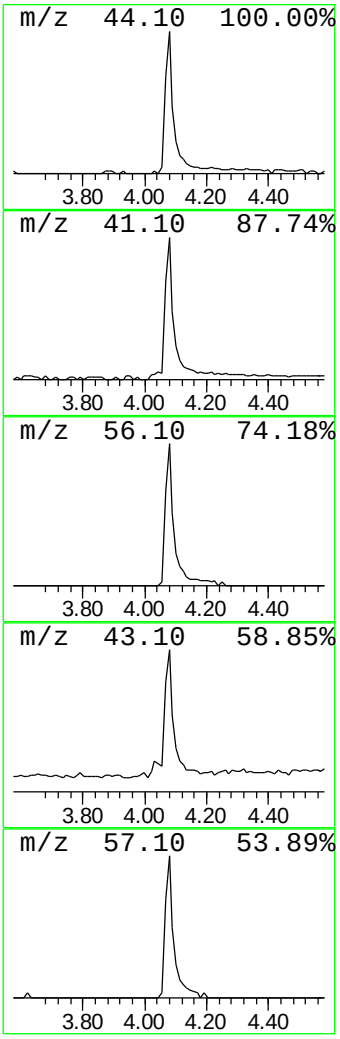
Peak Number 2 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	3.43 ng	165417	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	78
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	78
3	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
4	2-Butene, (E)-	56	C4H8	000624-64-6	27
5	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27





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Sample : H3052-01
Misc :
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Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

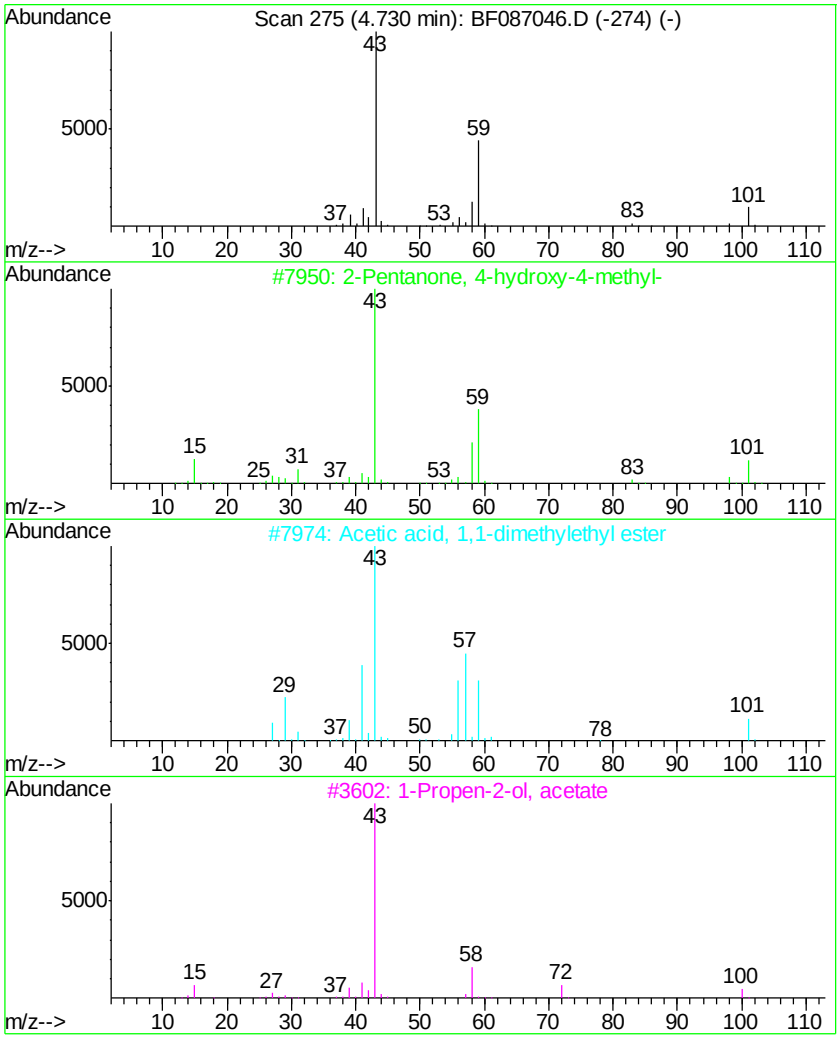
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

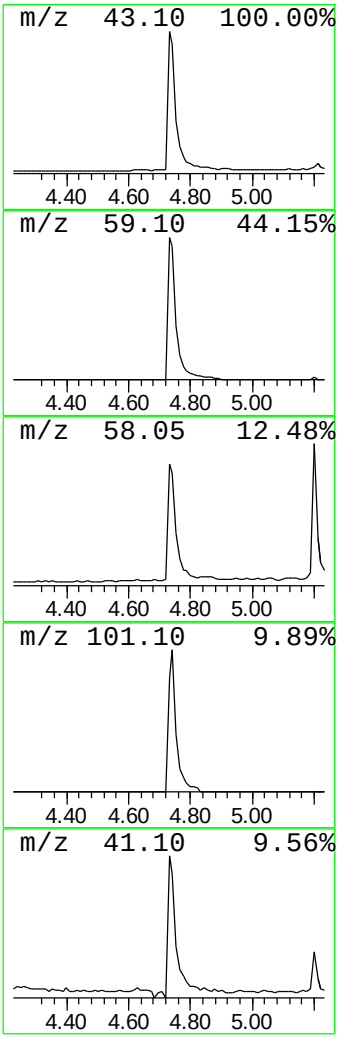
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	7.38 ng	355733	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane	58	C4H10	000106-97-8	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Sample : H3052-01
Misc :
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Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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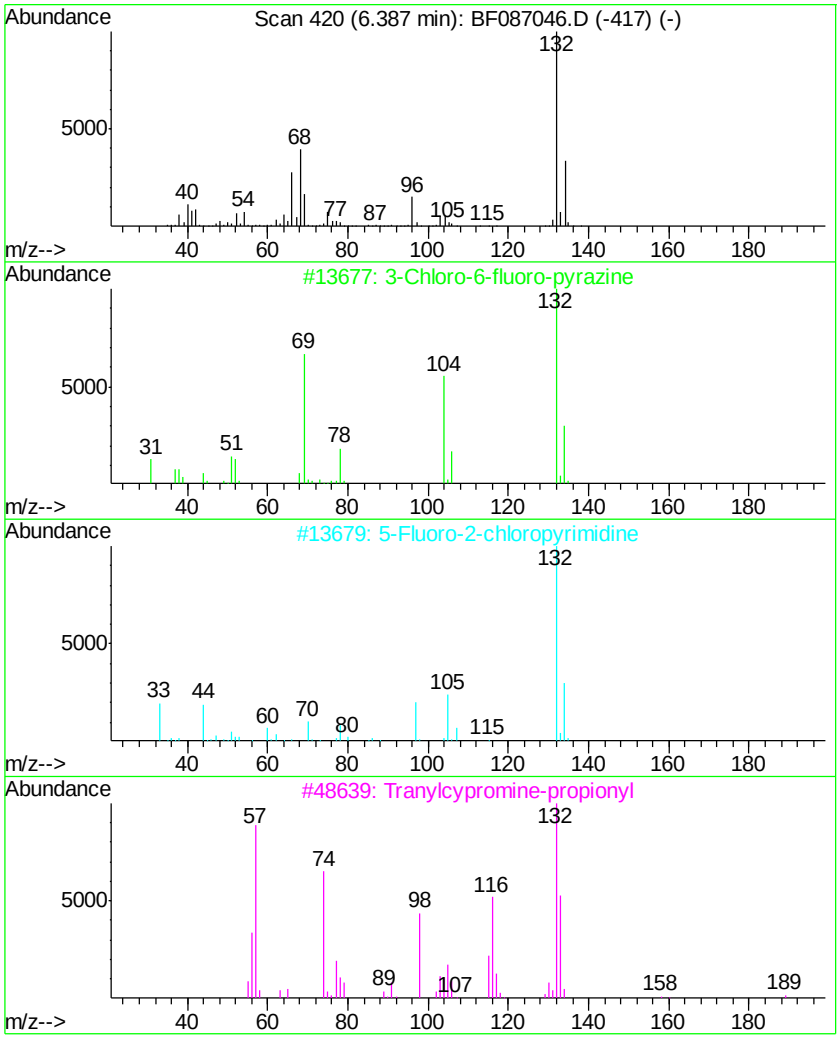
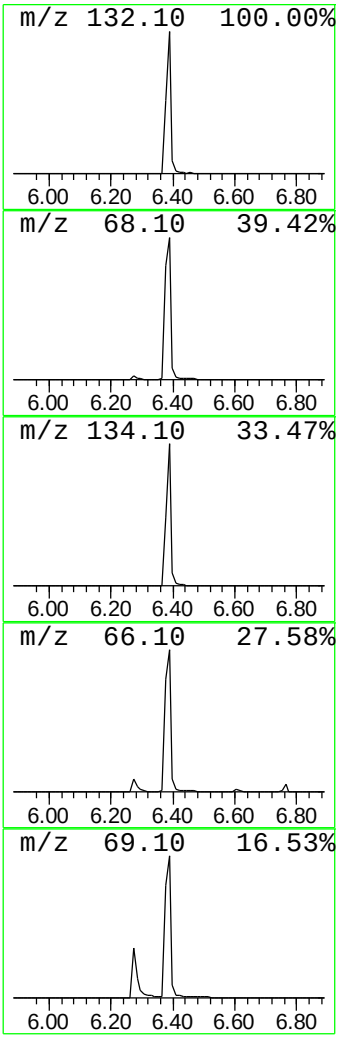
Peak Number 4 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	73.43 ng	3537840	1,4-Dichlorobenzene-d4	6.60

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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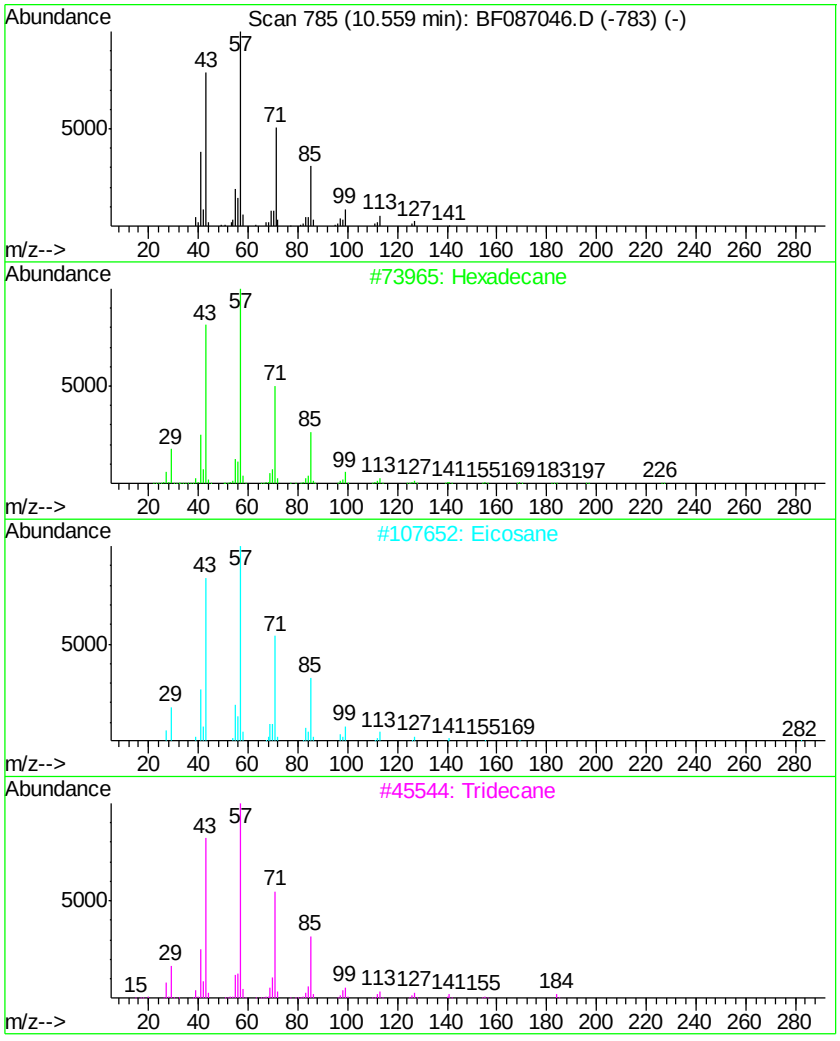
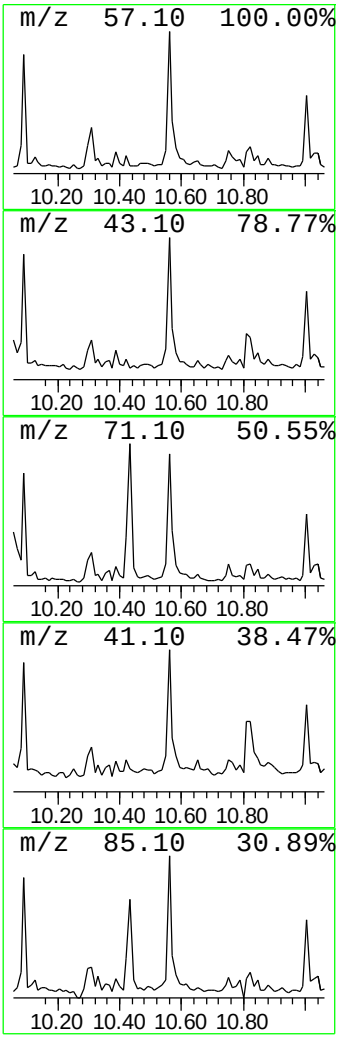
Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.07 ng	127063	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Heptadecane	240	C17H36	000629-78-7	80





Library Search Compound Report

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Operator : UM/SJ
Sample : H3052-01
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-24

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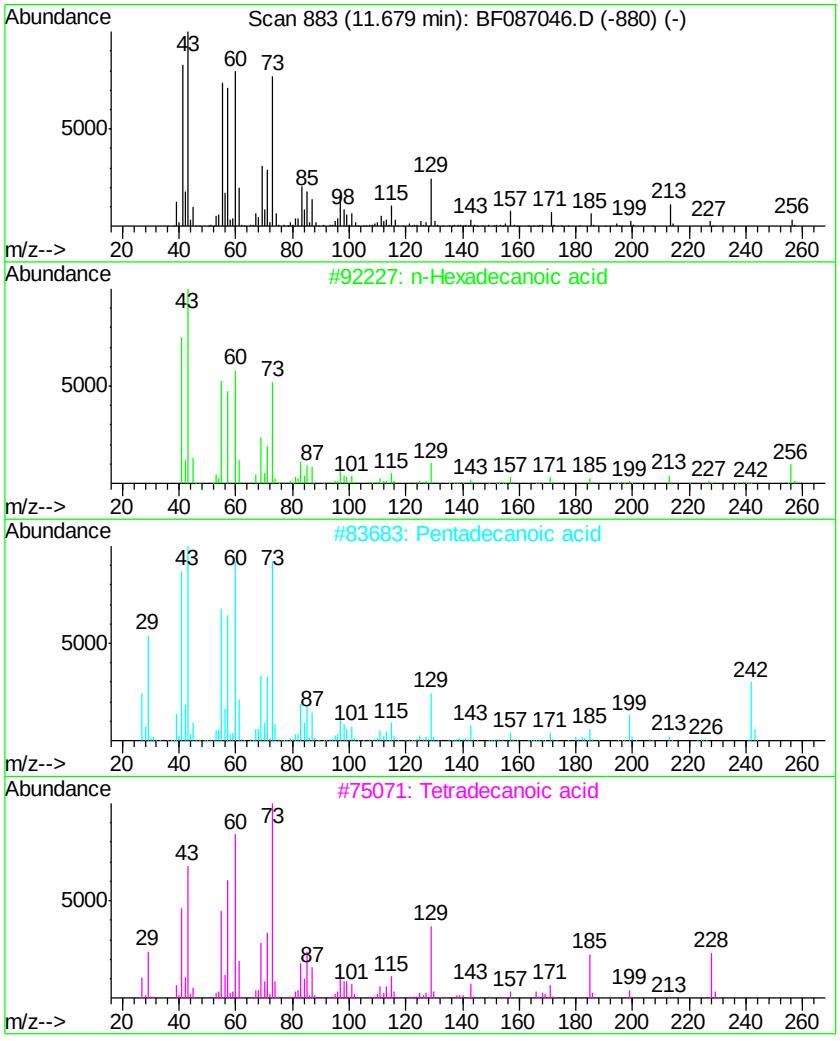
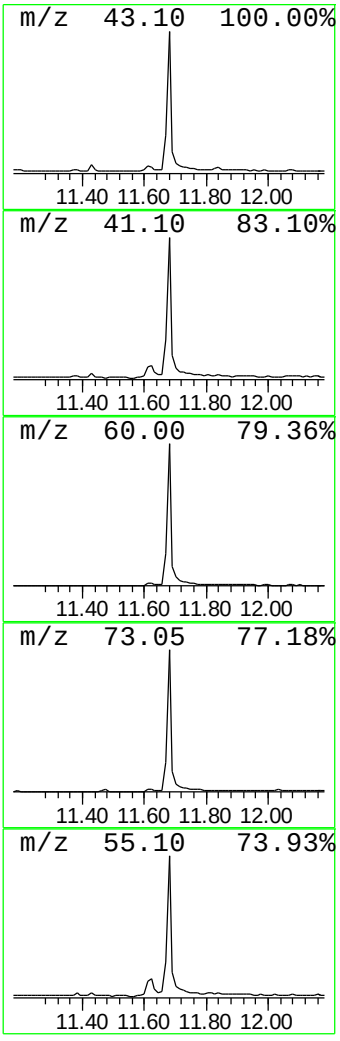
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	18.03 ng	1106630	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	78
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Sample : H3052-01
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Instrument : BNA_F
ClientSampleId : MW-24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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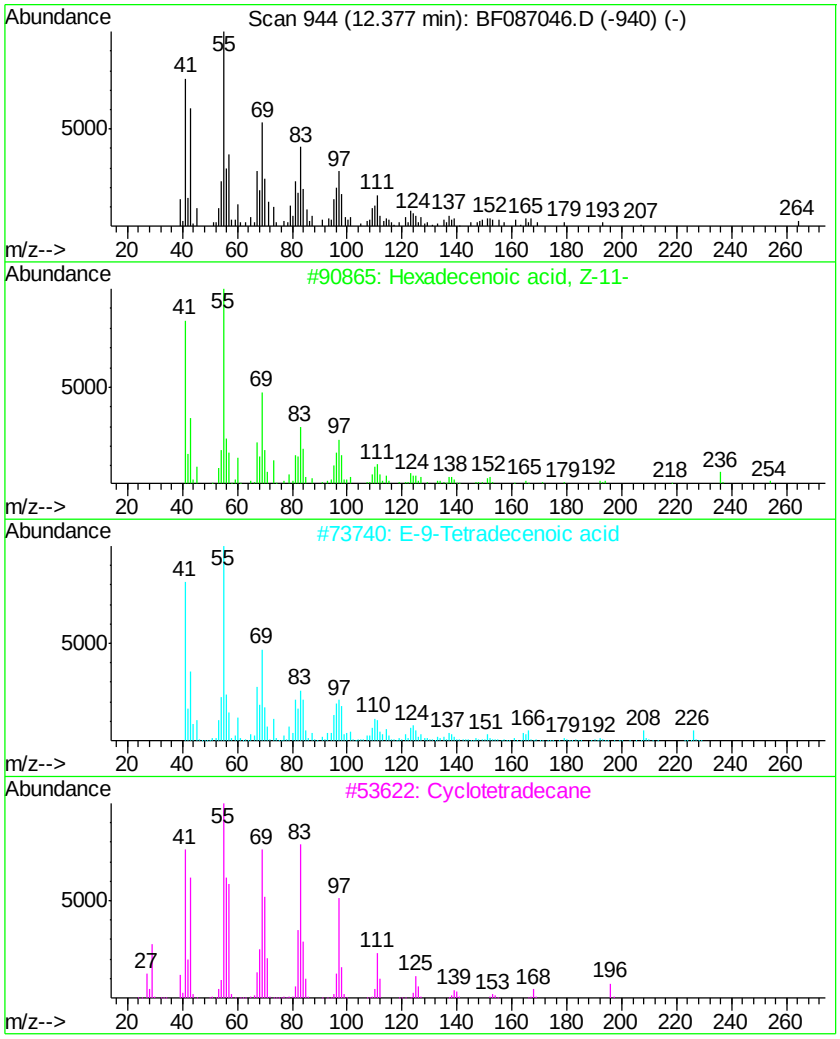
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

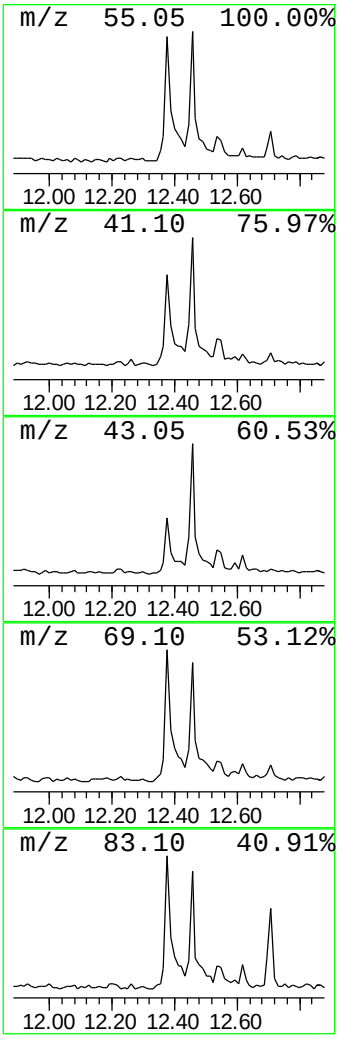
****

Peak Number 9 Hexadecenoic acid, Z-11- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	3.71 ng	227796	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	64
2	E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	58
3	Cyclotetradecane	196	C14H28	000295-17-0	52
4	Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	52
5	Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	52





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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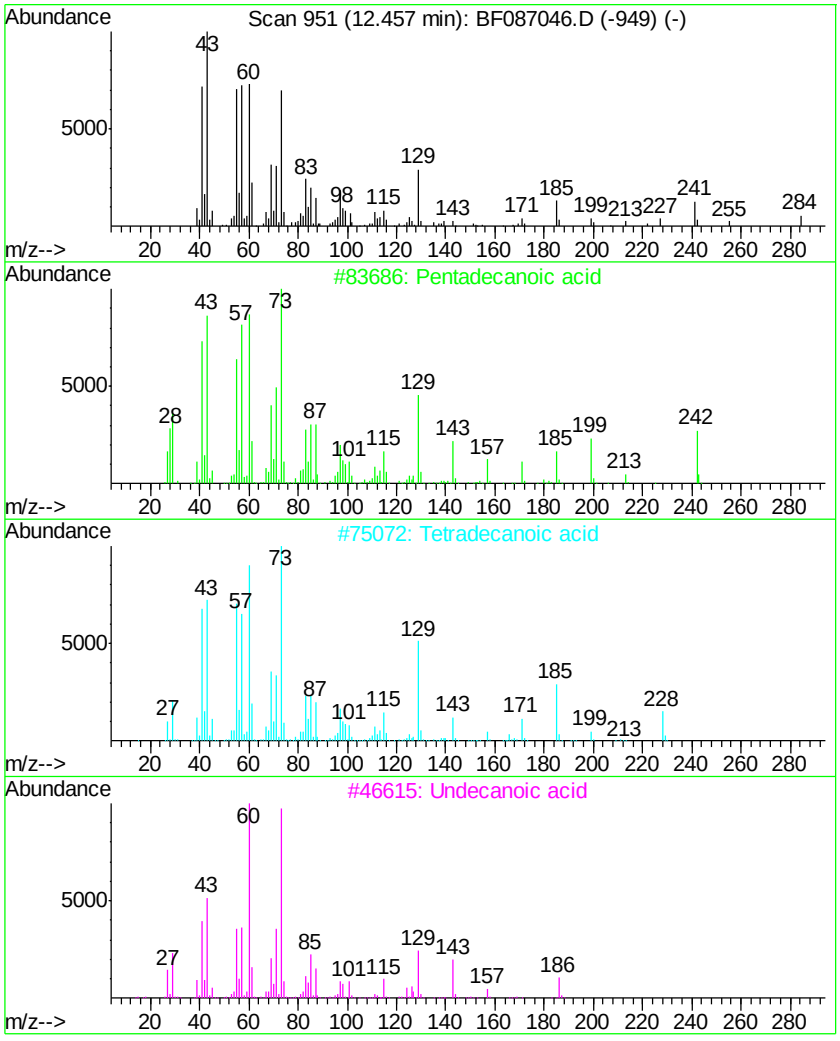
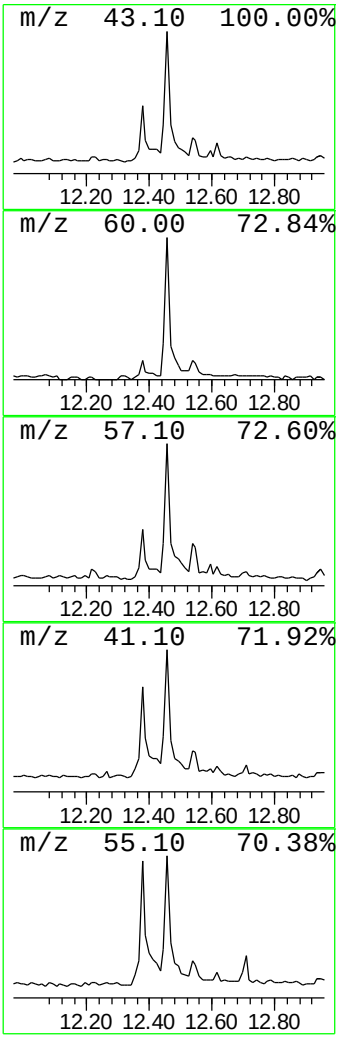
Peak Number 10 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	6.75 ng	325618	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	58
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
5	Lactose	342	C12H22O11	000063-42-3	47





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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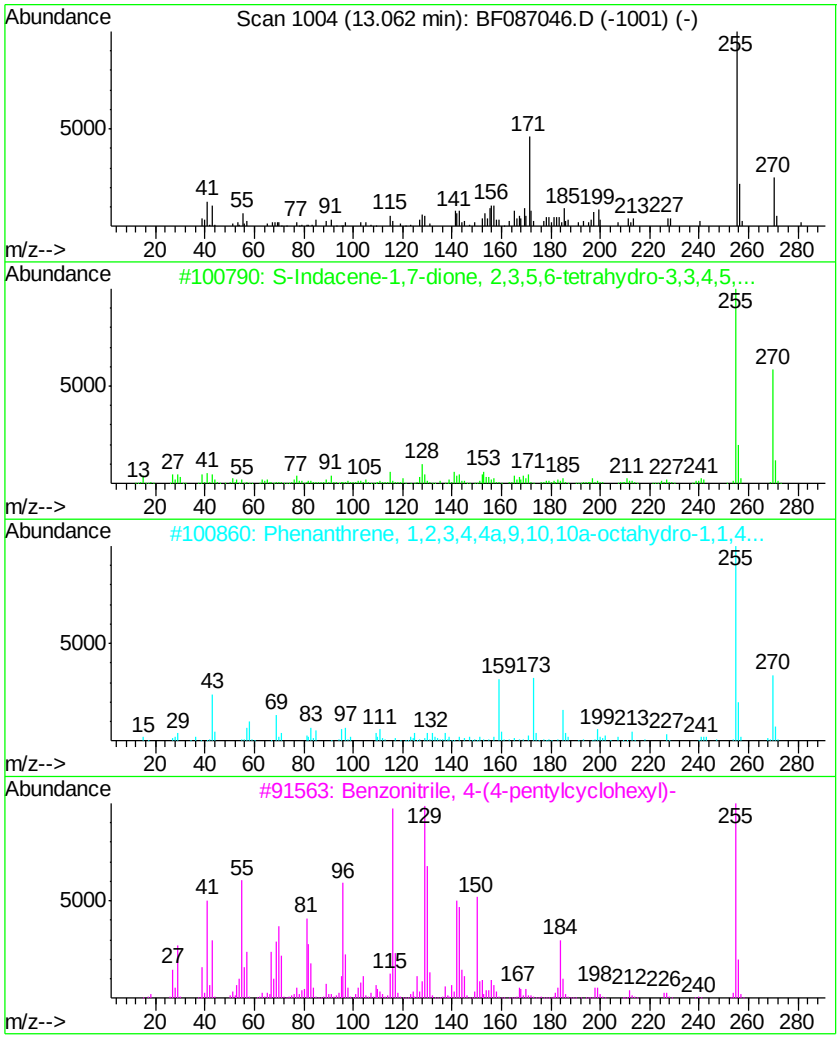
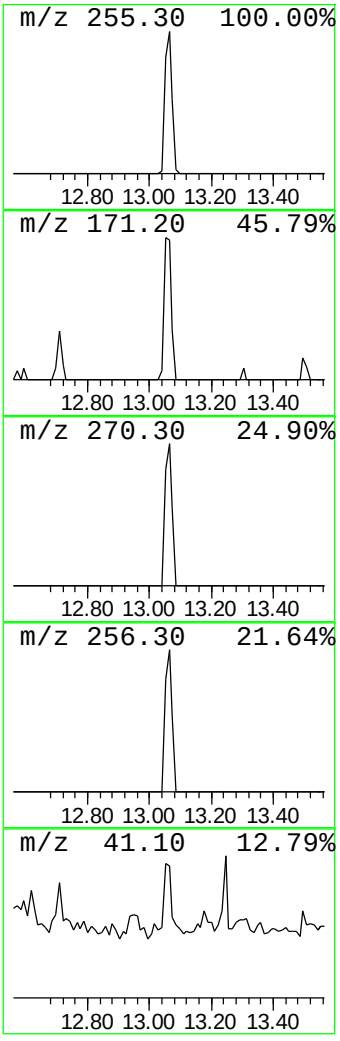
Peak Number 11 S-Indacene-1,7-dione, 2,3,5... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	2.68 ng	129249	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Indacene-1,7-dione, 2,3,5,6-te...	270	C18H22O2	055591-16-7	70
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	270	C20H30	019407-28-4	47
3	Benzonitrile, 4-(4-pentylcyclohe...	255	C18H25N	062788-05-0	46
4	2-(4-t-Butylphenoxy)benzoic acid	270	C17H18O3	069737-65-1	43
5	Iron, (.eta.-5-cyclohexadienyl)(...	270	C16H22Fe	1000162-99-3	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

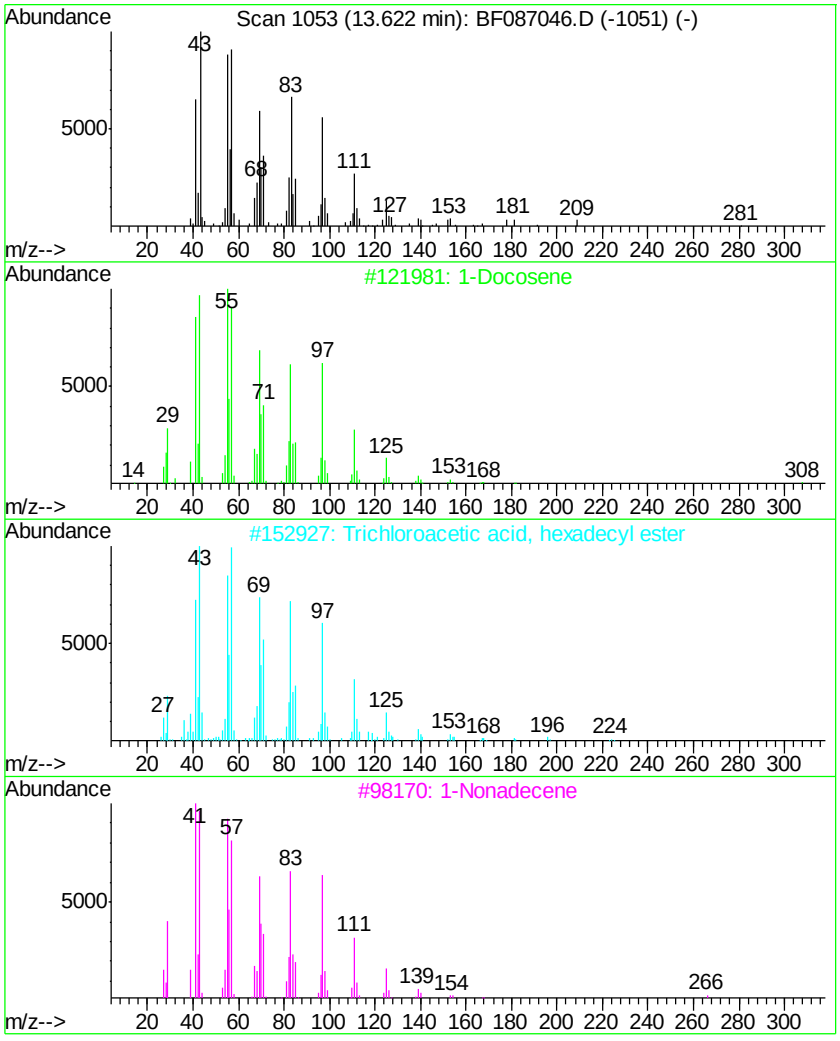
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

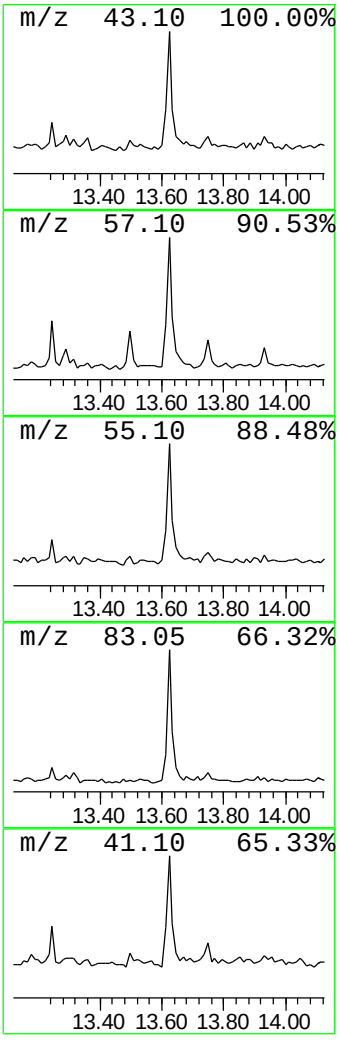
****

Peak Number 12 1-Docosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	2.58 ng	124318	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
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Acq On : 15 May 2016 3:56
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanal	4.08	3.4	ng	165417	1	6.60	963535	20.0
2-Pentanone, 4-hy...	4.73	7.4	ng	355733	1	6.60	963535	20.0
unknown6.39	6.39	73.4	ng	3537840	1	6.60	963535	20.0
Hexadecane	10.56	2.1	ng	127063	4	11.12	1227450	20.0
n-Hexadecanoic acid	11.68	18.0	ng	1106630	4	11.12	1227450	20.0
Hexadecenoic acid...	12.38	3.7	ng	227796	4	11.12	1227450	20.0
Pentadecanoic acid	12.46	6.8	ng	325618	5	13.75	964730	20.0
S-Indacene-1,7-di...	13.06	2.7	ng	129249	5	13.75	964730	20.0
1-Docosene	13.62	2.6	ng	124318	5	13.75	964730	20.0