LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111716\
Data File : BF091229.D
Acq On : 17 Nov 2016 23:00
Operator : UM/SJ
Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

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-BF110316.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	2.681	84	87	96	rVB	43187	94896	1.76%	0.225%
2	4.738	265	267	277	rBV	451383	602875	11.19%	1.427%
3	5.196	305	307	321	rBV	1441346	2125387	39.45%	5.032%
4	6.270	399	401	409	rBV	895457	1235672	22.93%	2.926%
5	6.384	409	411	414	rBV	2961464	3147506	58.42%	7.453%
6	6.613	429	431	437	rBV	854028	1086432	20.16%	2.572%
7	6.773	442	445	448	rBV	3505949	3360859	62.37%	7.958%
8	7.059	466	470	476	rVB5	30673	66309	1.23%	0.157%
9	7.196	479	482	484	rBV	2640148	3001007	55.70%	7.106%
10	7.367	491	497	499	rBV	261371	613040	11.38%	1.452%
11	7.824	535	537	542	rBV2	63095	106458	1.98%	0.252%
12	7.904	542	544	547	rBV	1498802	1469683	27.28%	3.480%
13	8.190	567	569	573	rVB2	67276	98496	1.83%	0.233%
14	8.705	611	614	616	rBV	580872	572088	10.62%	1.355%
15	8.876	625	629	631	rBV2	51675	85584	1.59%	0.203%
16	8.990	636	639	642	rBV	5312344	5388155	100.00%	12.758%
17	9.390	672	674	676	rBV	125112	103680	1.92%	0.245%
18	9.436	676	678	686	rVB	905765	893246	16.58%	2.115%
19	9.585	690	691	695	rVB2	35674	63065	1.17%	0.149%
20	9.653	695	697	700	rBV	1413671	1677048	31.12%	3.971%
21	9.928	717	721	723	rBV3	25427	61541	1.14%	0.146%
22	10.099	730	736	738	rBV4	47764	119243	2.21%	0.282%
23	10.396	759	762	764	rBV3	46903	99697	1.85%	0.236%
24	10.453	764	767	769	rBV	3043246	3353475	62.24%	7.940%
25	10.579	776	778	781	rBV2	91066	126737	2.35%	0.300%
26	10.785	793	796	801	rVB	366736	451429	8.38%	1.069%
27	11.025	812	817	824	rBV3	122886	386886	7.18%	0.916%
28	11.139	824	827	829	rBV	2044814	1816038	33.70%	4.300%
29	11.333	840	844	847	rBV5	28684	78896	1.46%	0.187%
30	11.448	852	854	856	rBV	65150	66860	1.24%	0.158%
31	11.608	866	868	873	rBV3	28165	75753	1.41%	0.179%
32	11.688	873	875	876	rBV	46362	55871	1.04%	0.132%
33	11.859	888	890	891	rBV	61824	79890	1.48%	0.189%
34	11.951	896	898	899	rBV	87813	128790	2.39%	0.305%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : WQ-5W

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-BF110316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.133	912	914	916	rBV2	45915	66649	1.24%	0.158%
36	12.248	921	924	925	rBV	75082	87869	1.63%	0.208%
37	12.282	925	927	931	rVB	36522	59546	1.11%	0.141%
38	12.351	931	933	934	rBV2	36383	56991	1.06%	0.135%
39	12.385	934	936	937	rBV	54740	59718	1.11%	0.141%
40	12.488	943	945	946	rBV	48571	80466	1.49%	0.191%
41	12.613	955	956	958	rBV2	117062	136995	2.54%	0.324%
42	12.728	963	966	969	rBV	5007463	5349702	99.29%	12.667%
43	12.968	985	987	988	rBV2	82396	85835	1.59%	0.203%
44	13.094	996	998	1000	rBV	103842	149700	2.78%	0.354%
45	13.311	1014	1017	1018	rBV2	148870	196157	3.64%	0.464%
46	13.642	1044	1046	1053	rVB2	148203	332760	6.18%	0.788%
47	13.768	1055	1057	1060	rVB	1150248	1301308	24.15%	3.081%
48	14.259	1098	1100	1104	rVB3	159485	293280	5.44%	0.694%
49	14.557	1124	1126	1128	rVB	135521	140967	2.62%	0.334%
50	14.854	1150	1152	1153	rVB	127681	121768	2.26%	0.288%
51	15.139	1175	1177	1180	rBV	650548	897823	16.66%	2.126%
52	15.551	1211	1213	1215	rBV	84493	123919	2.30%	0.293%

Sum of corrected areas: 42234045

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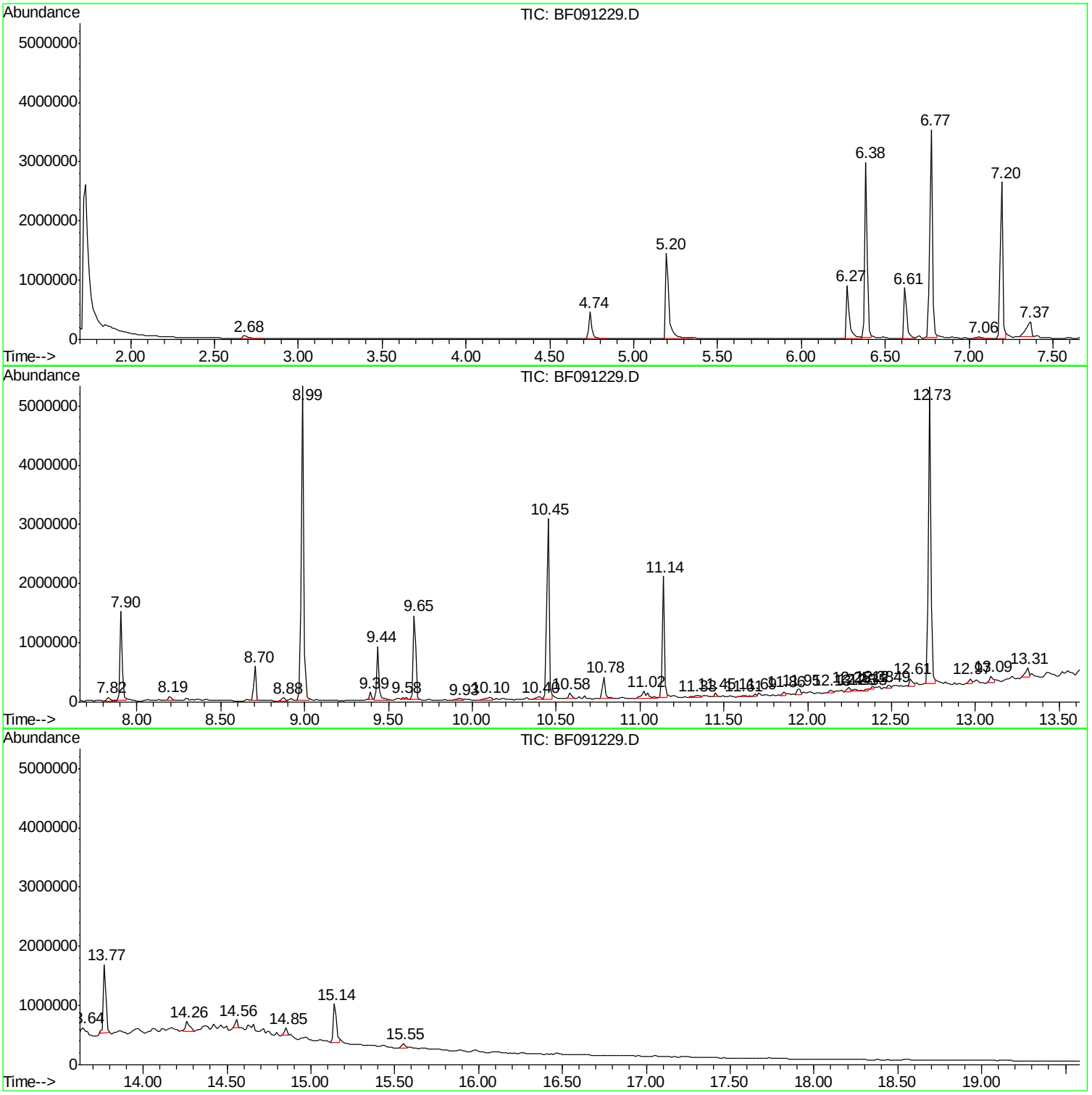
BNA_F
ClientSampleId :
WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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\BF111716\
Data File : BF091229.D
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Operator : UM/SJ
Sample : H5681-05
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Instrument : BNA_F
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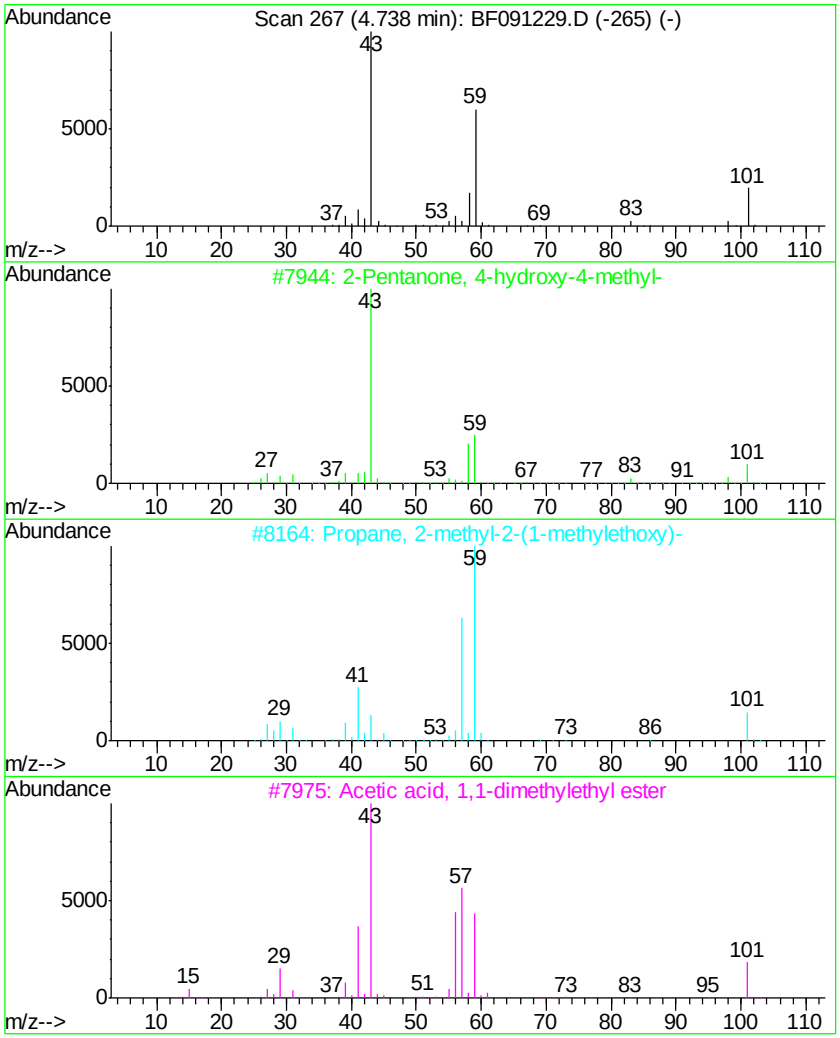
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

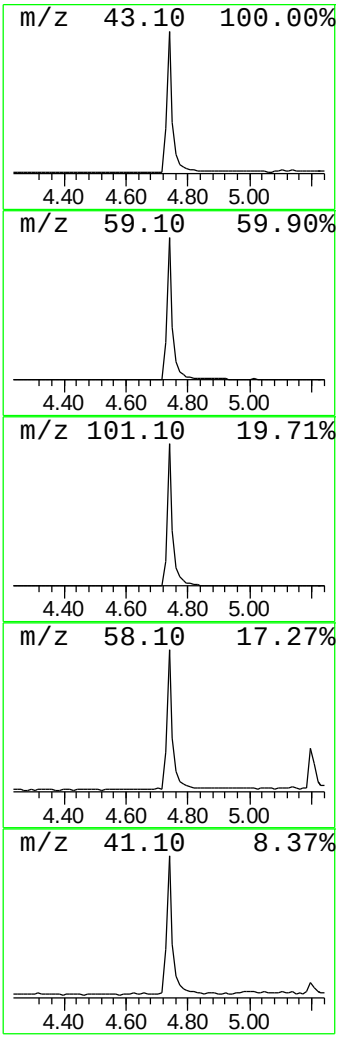
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	11.10 ng	602875	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : H5681-05
Misc :
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Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

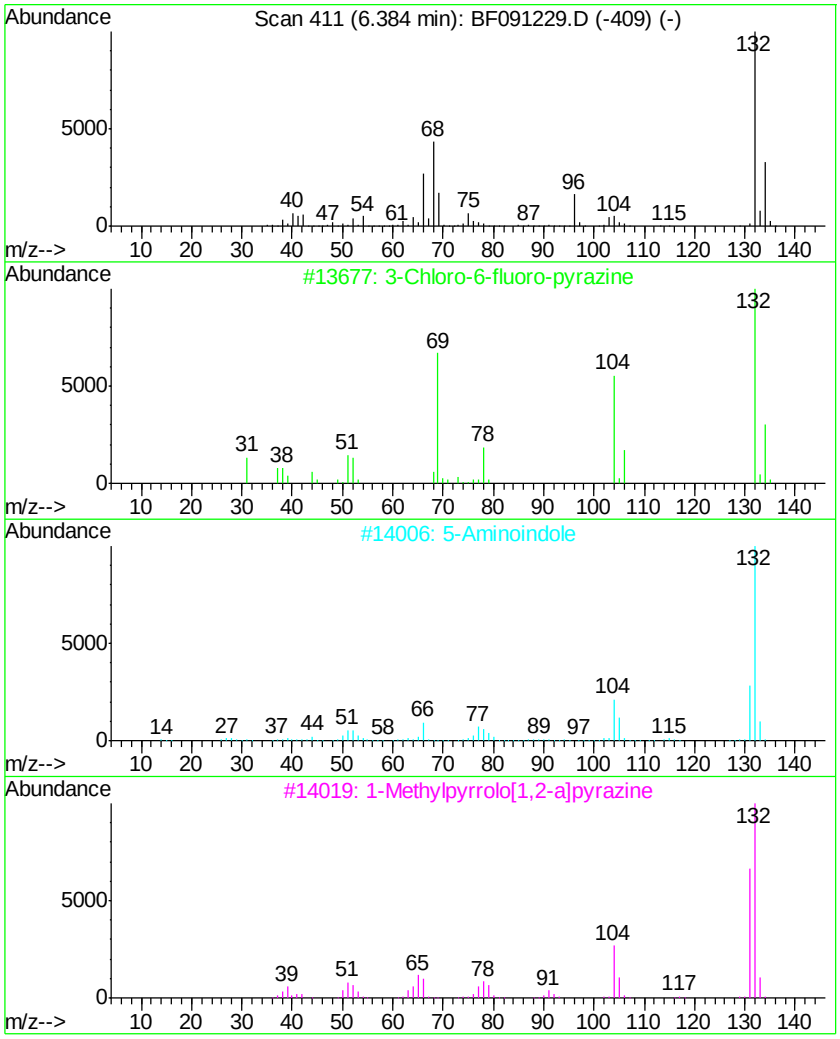
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

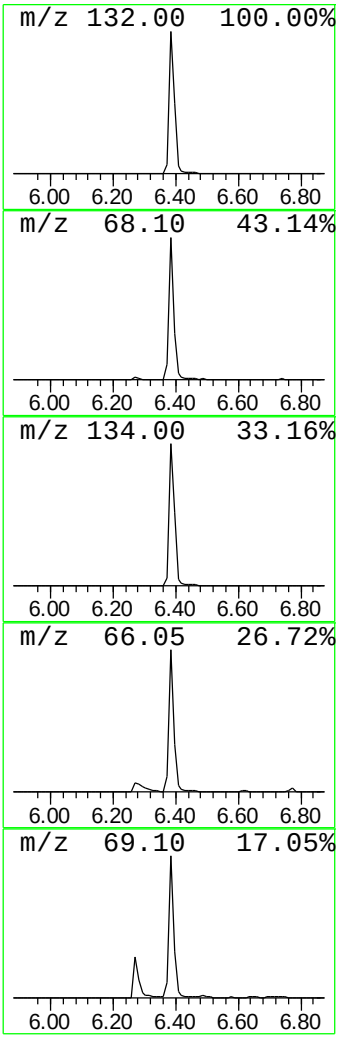
****

Peak Number 2 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	57.94 ng	3147510	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Sample : H5681-05
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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TIC Library : C:\DATABASE\NIST02.L
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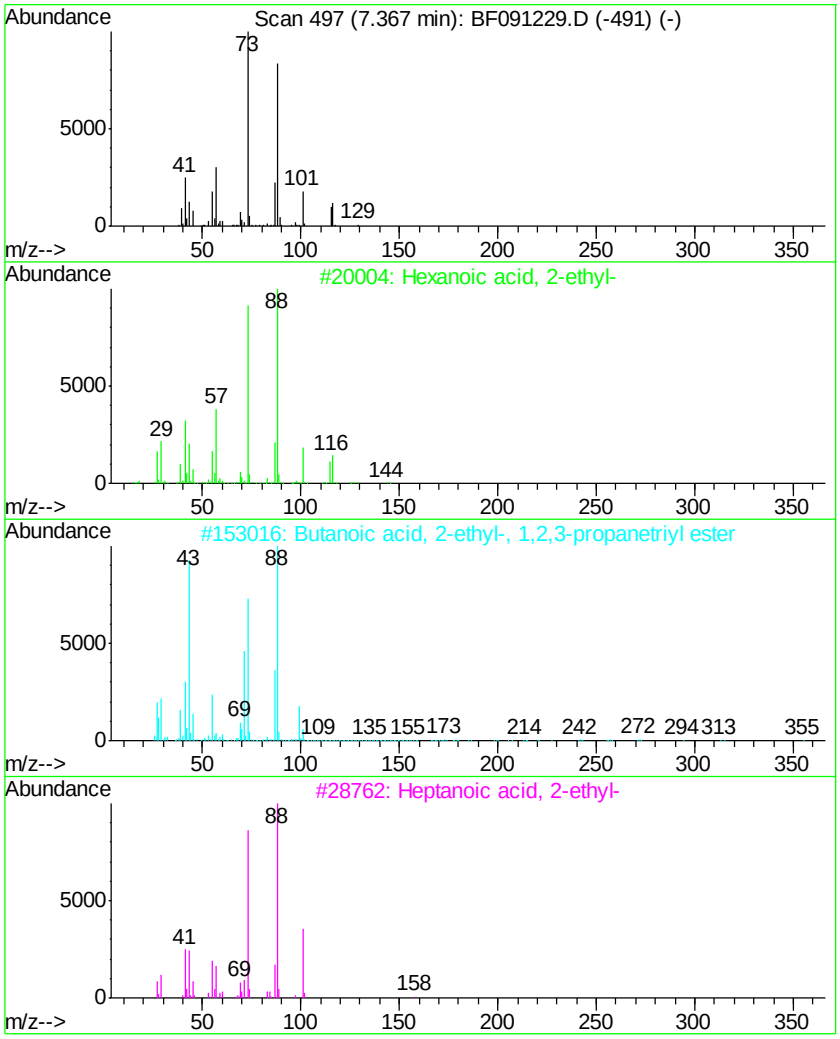
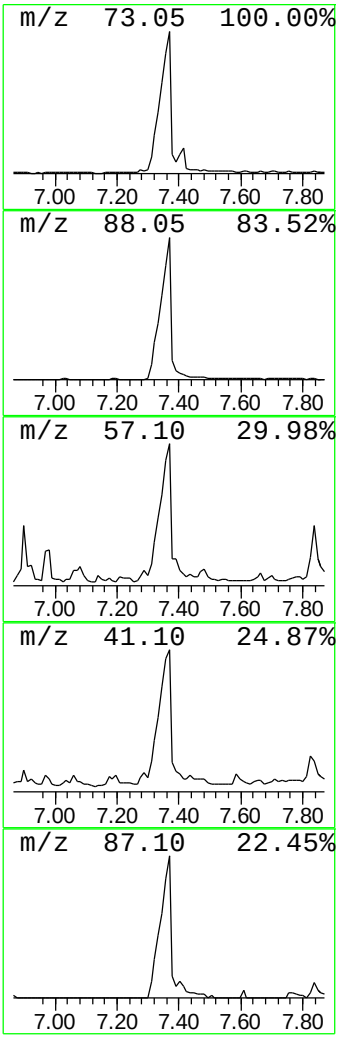
****

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	8.34 ng	613040	Naphthalene-d8	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	50
4	1,4-Dioxane	88	C4H8O2	000123-91-1	37
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	28





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Sample : H5681-05
Misc :
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Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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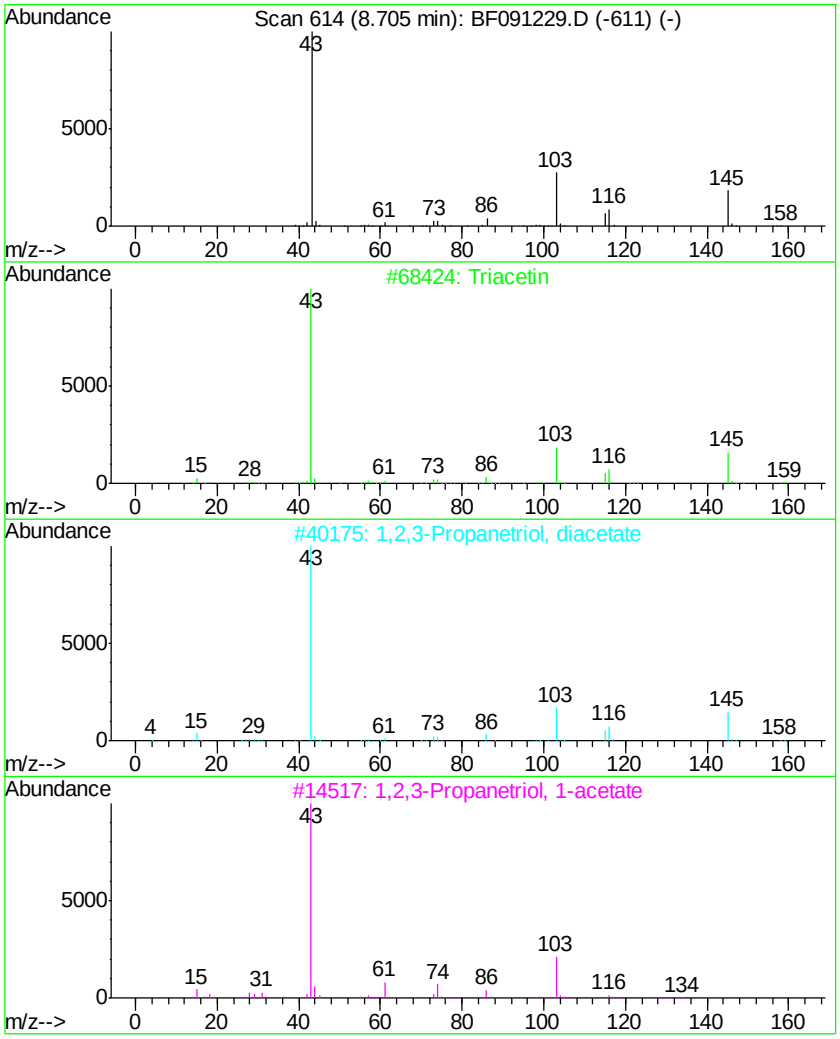
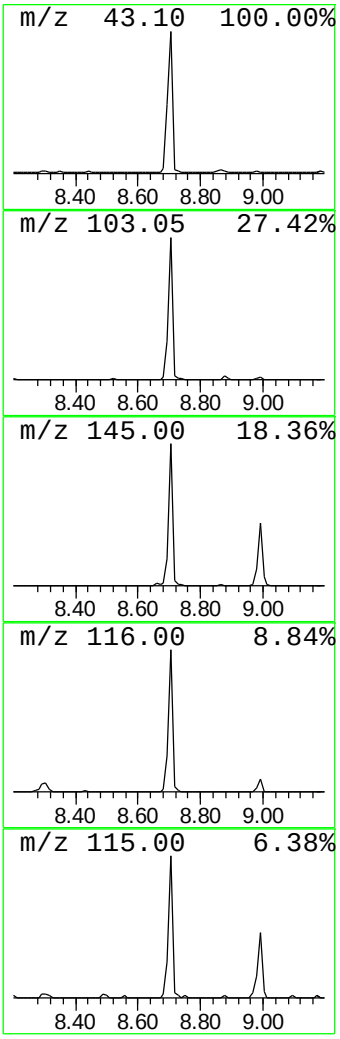
****

Peak Number 5 Triacetin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	7.79 ng	572088	Naphthalene-d8	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacetin	218	C9H14O6	000102-76-1	83
2	1,2,3-Propanetriol, diacetate	176	C7H12O5	025395-31-7	83
3	1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	36
4	1,2,3-Propanetriol, monoacetate	134	C5H10O4	026446-35-5	9
5	Propanoic acid, 2-oxo-, ethyl ester	116	C5H8O3	000617-35-6	7





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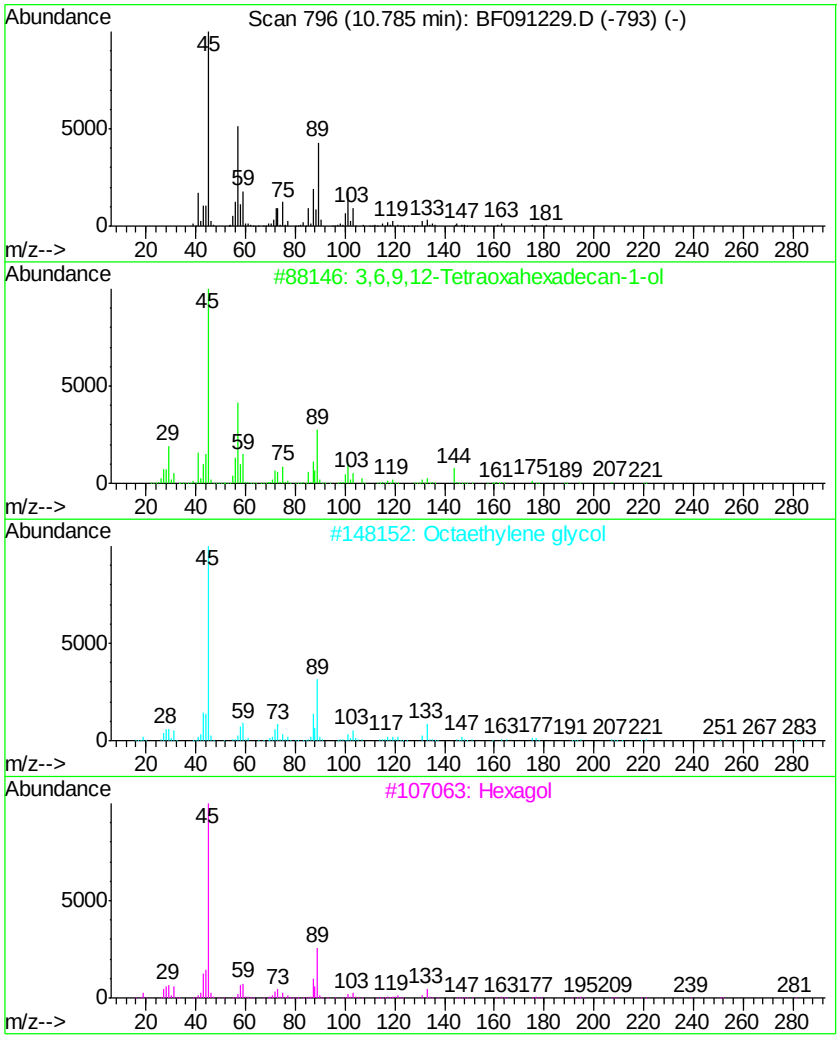
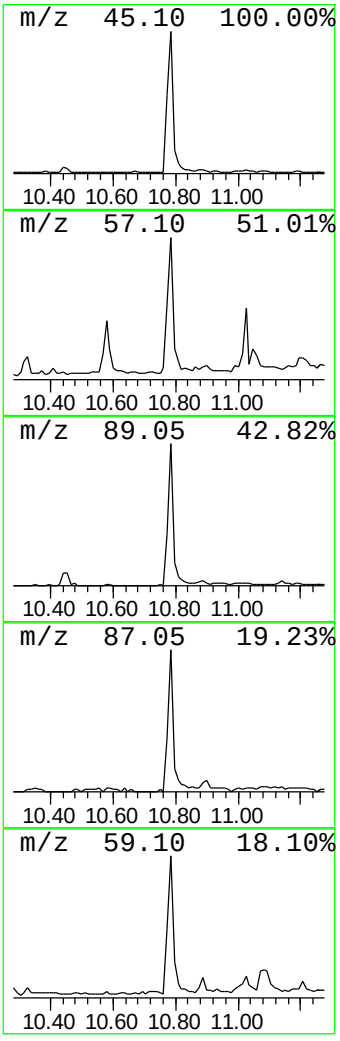
****

Peak Number 6 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	4.97 ng	451429	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	90
2	Octaethylene glycol	370	C16H34O9	1000289-34-2	86
3	Hexagol	282	C12H26O7	002615-15-8	72
4	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	59
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	52





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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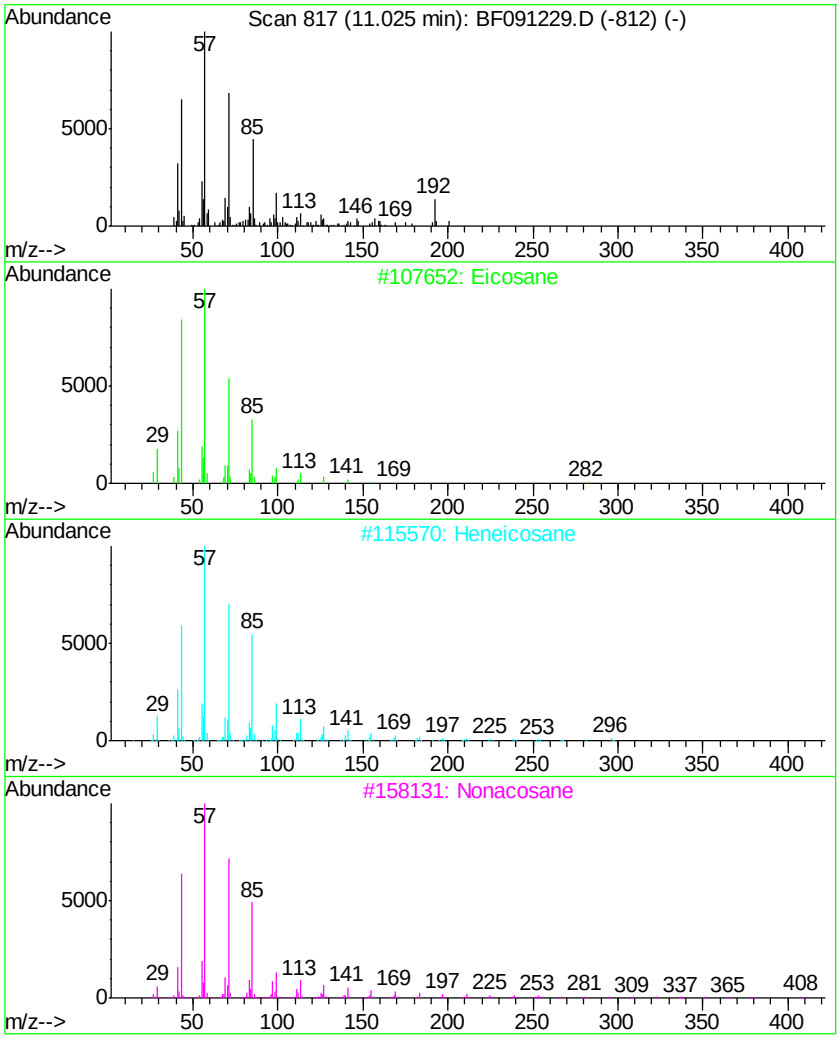
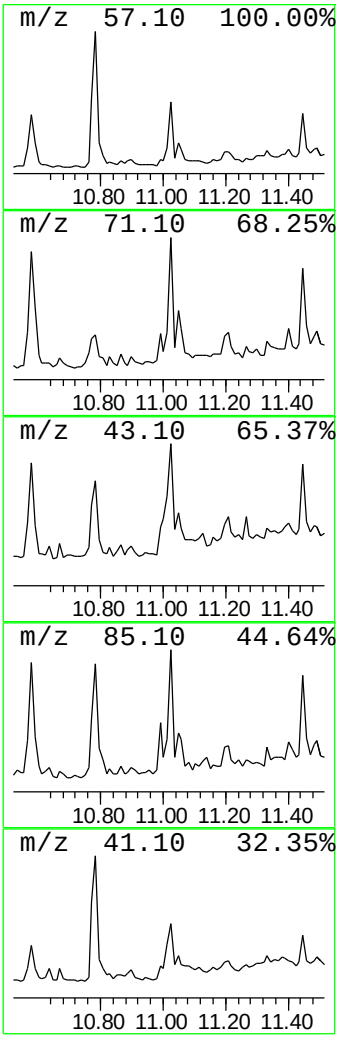
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	4.26 ng	386886	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	74
2	Heneicosane	296	C21H44	000629-94-7	74
3	Nonacosane	408	C29H60	000630-03-5	72
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
5	Heptacosane	380	C27H56	000593-49-7	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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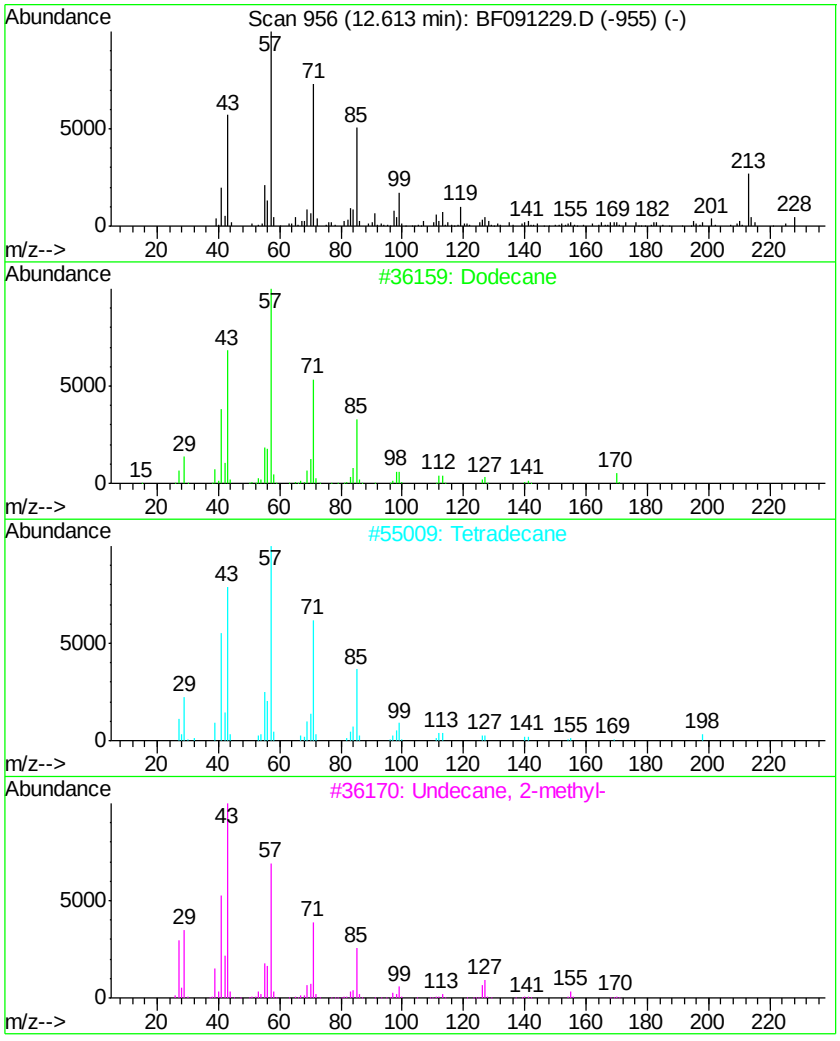
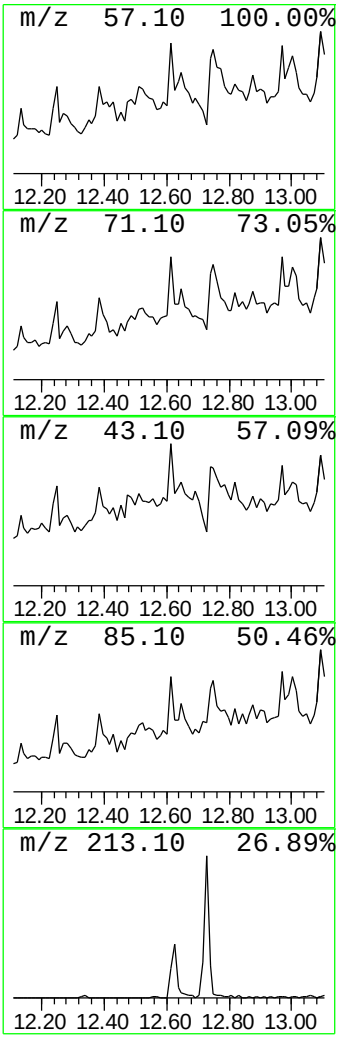
Peak Number 8 Dodecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	2.11 ng	136995	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	62
2	Tetradecane	198	C14H30	000629-59-4	58
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	58
4	Heneicosane	296	C21H44	000629-94-7	58
5	Hexadecane	226	C16H34	000544-76-3	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111716\
Data File : BF091229.D
Acq On : 17 Nov 2016 23:00
Operator : UM/SJ
Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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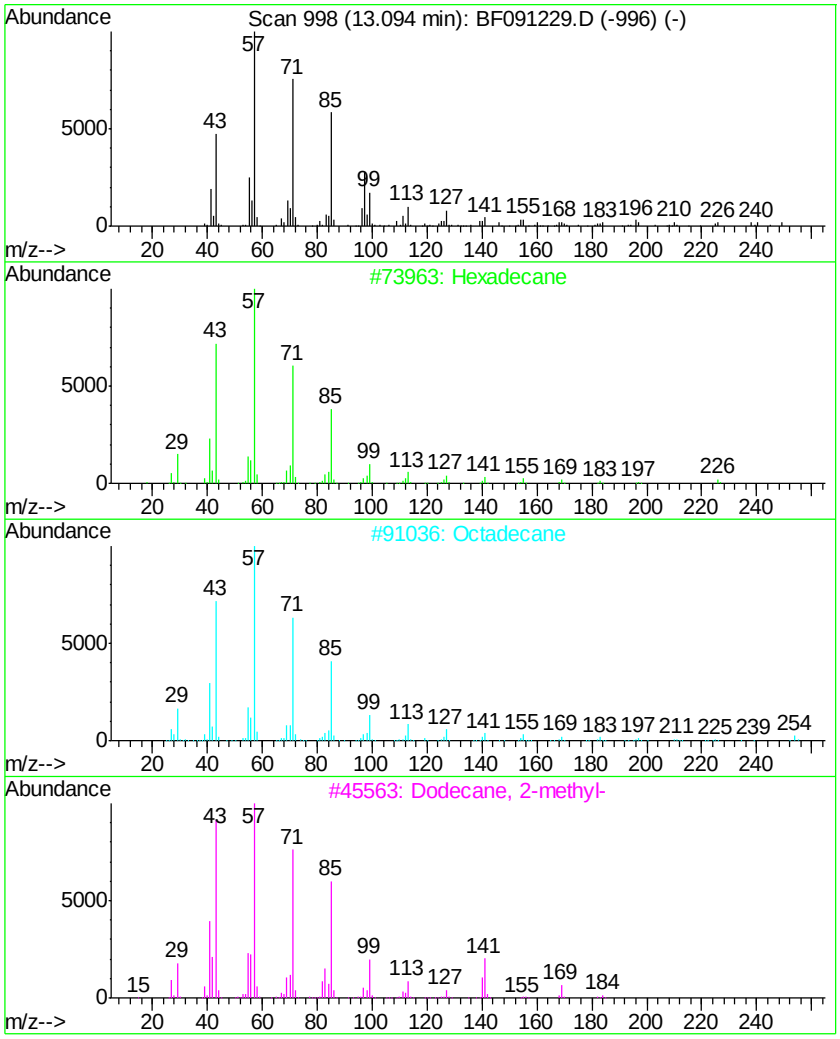
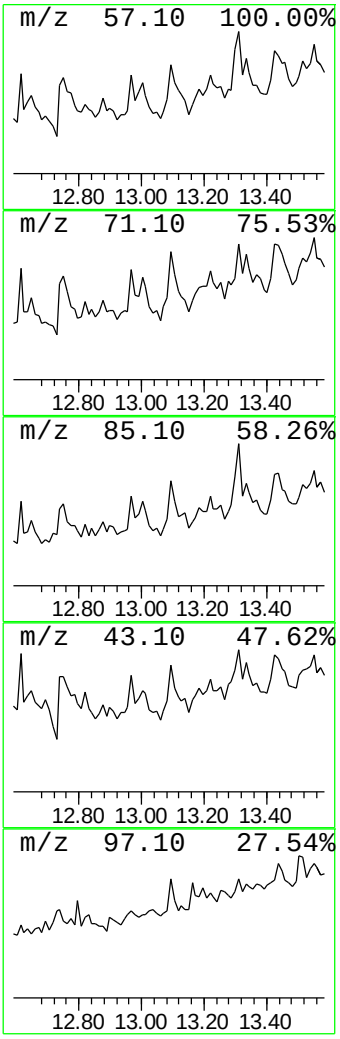
Peak Number 9 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	2.30 ng	149700	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	92
2	Octadecane	254	C18H38	000593-45-3	74
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	74
4	Tetracosane	338	C24H50	000646-31-1	72
5	Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	72





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Data File : BF091229.D
Acq On : 17 Nov 2016 23:00
Operator : UM/SJ
Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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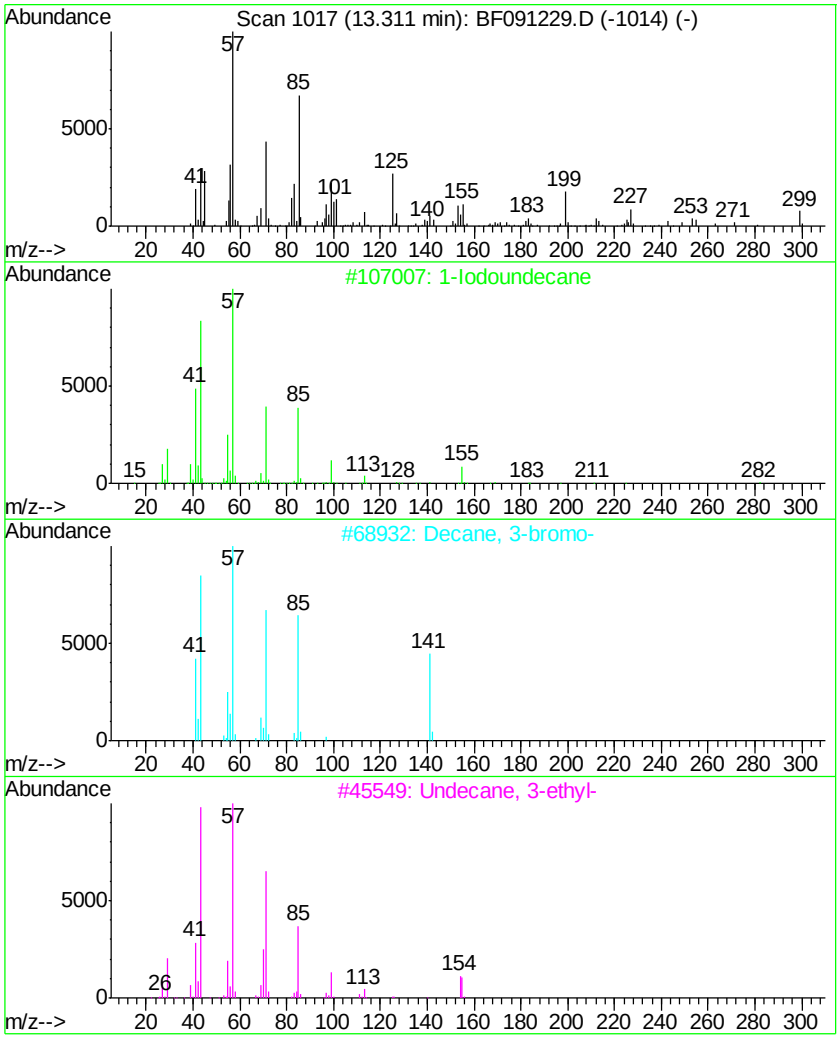
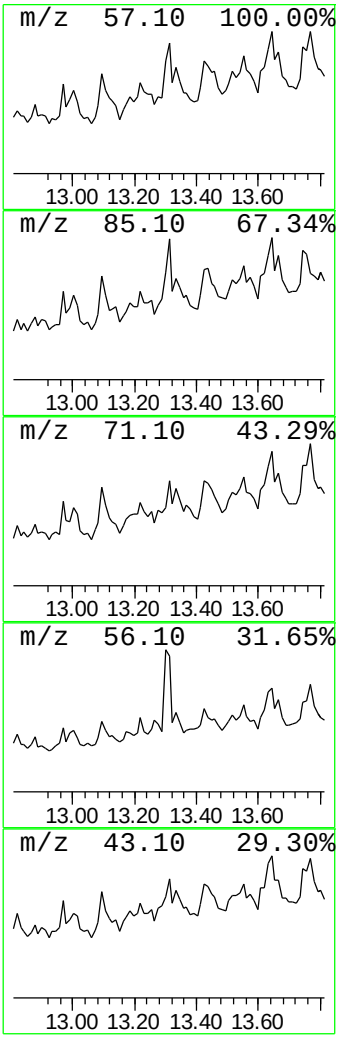
Peak Number 10 unknown13.31 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	3.01 ng	196157	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane	282	C11H23I	004282-44-4	43
2	Decane, 3-bromo-	220	C10H21Br	030571-71-2	35
3	Undecane, 3-ethyl-	184	C13H28	017312-58-2	35
4	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	30
5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	27





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Operator : UM/SJ
Sample : H5681-05
Misc :
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Instrument : BNA_F
ClientSampleId : WQ-5W

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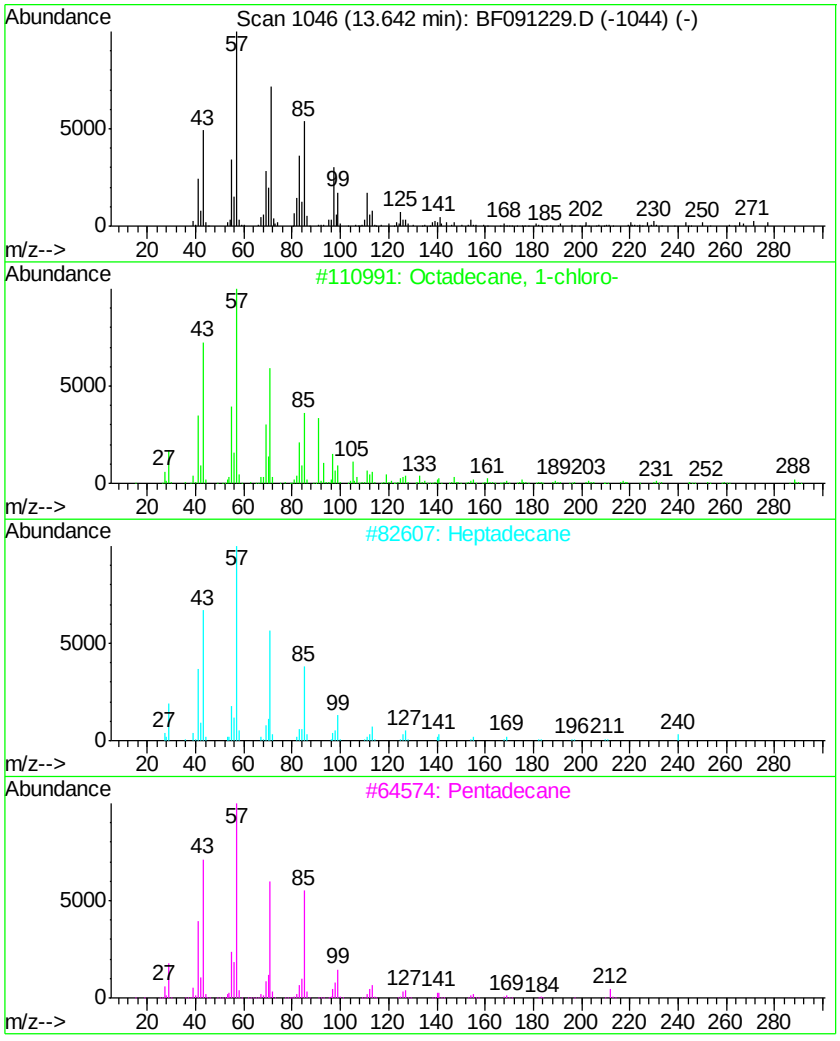
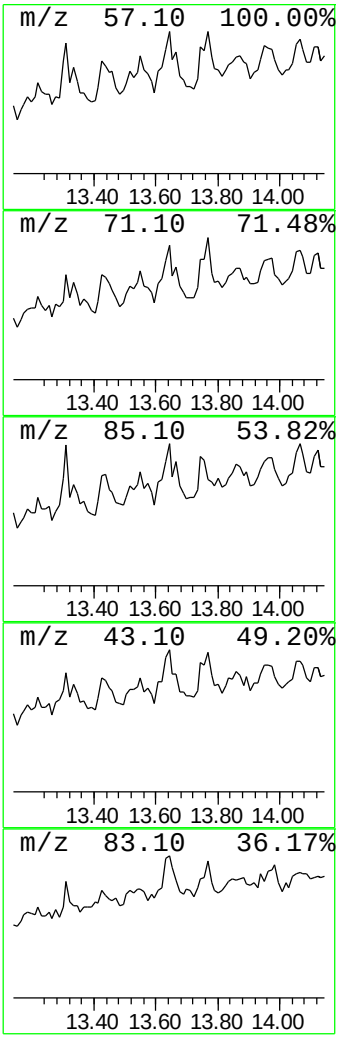
Peak Number 11 Octadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	5.11 ng	332760	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	59
2	Heptadecane	240	C17H36	000629-78-7	53
3	Pentadecane	212	C15H32	000629-62-9	52
4	4,4-Dipropylheptane	184	C13H28	017312-72-0	50
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50





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Operator : UM/SJ
Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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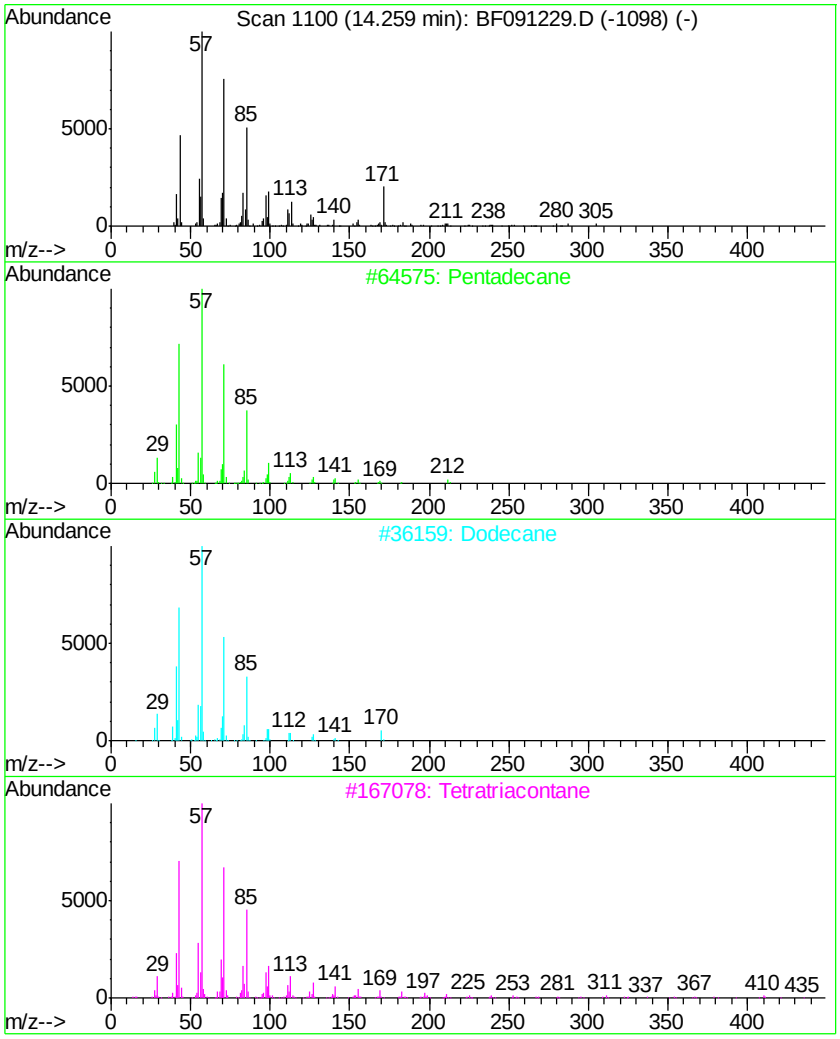
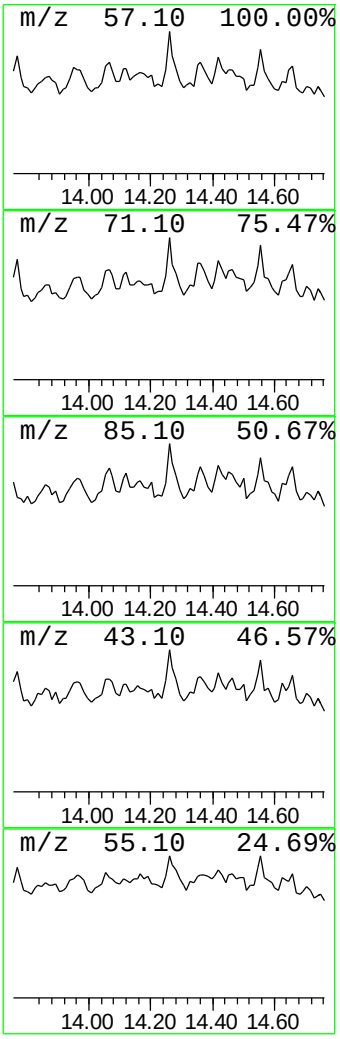
Peak Number 12 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	4.51 ng	293280	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Dodecane	170	C12H26	000112-40-3	81
3	Tetratriacontane	479	C34H70	014167-59-0	80
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5	Heptadecane	240	C17H36	000629-78-7	74





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Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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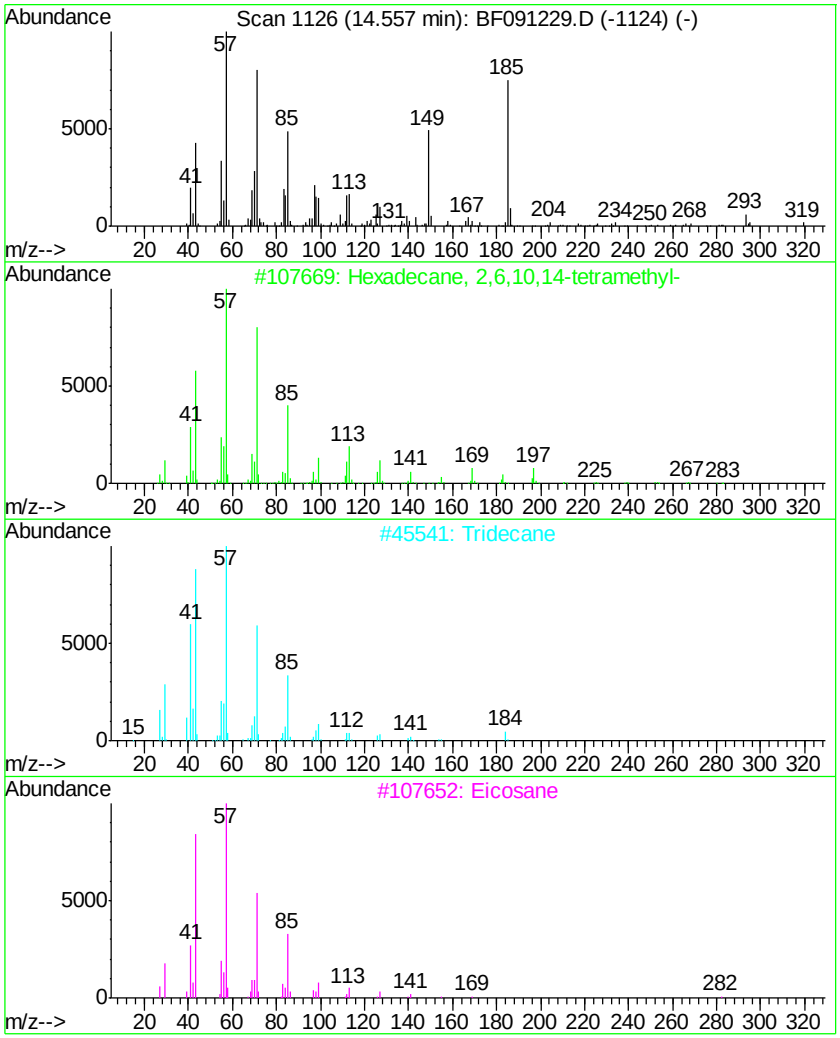
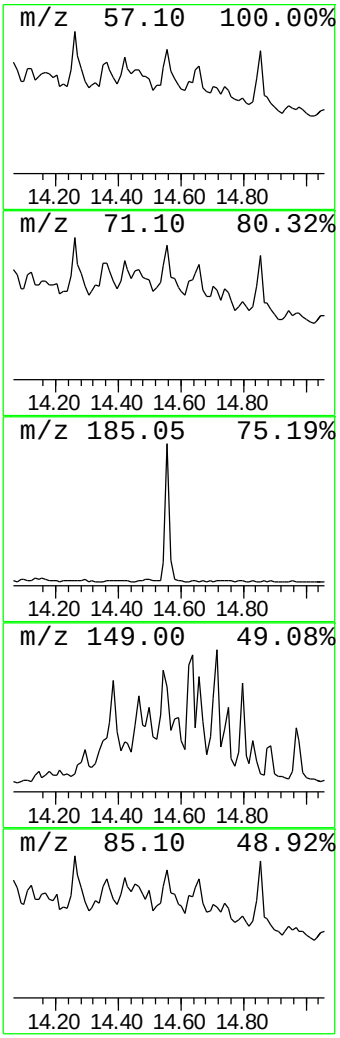
Peak Number 13 unknown14.56 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.14 ng	140967	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	46
2	Tridecane	184	C13H28	000629-50-5	46
3	Eicosane	282	C20H42	000112-95-8	45
4	Pentadecane	212	C15H32	000629-62-9	41
5	Hexadecane	226	C16H34	000544-76-3	41





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Sample : H5681-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WQ-5W

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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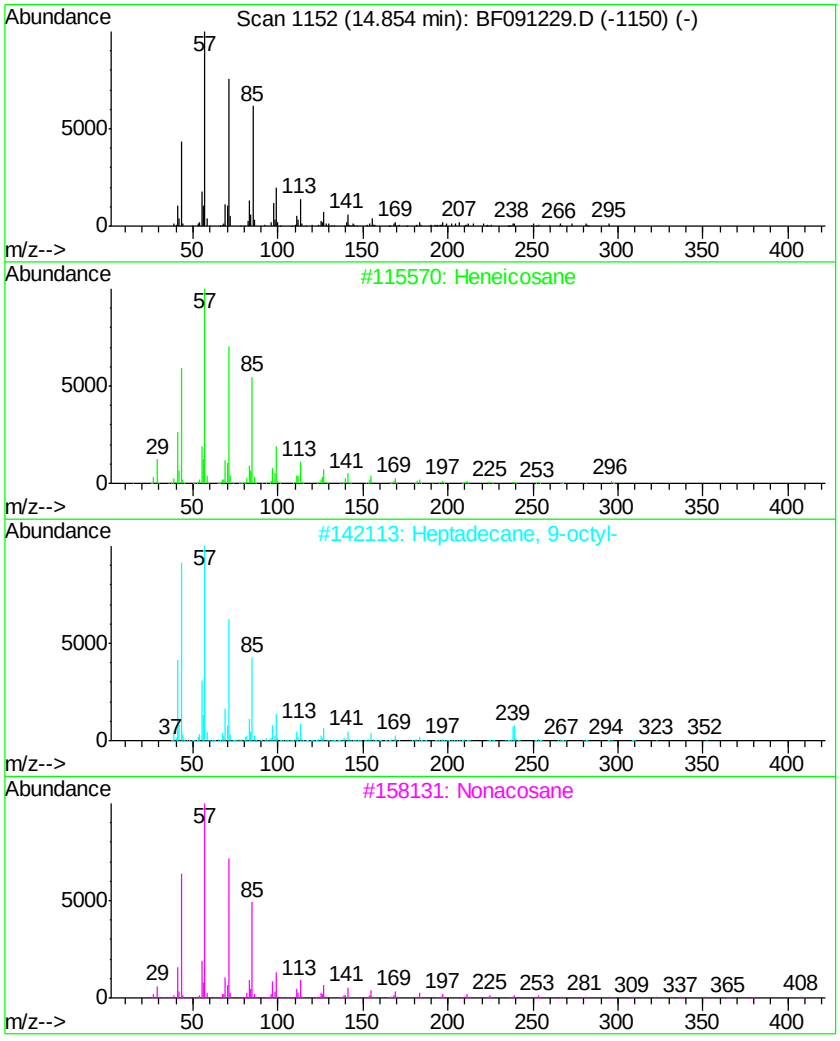
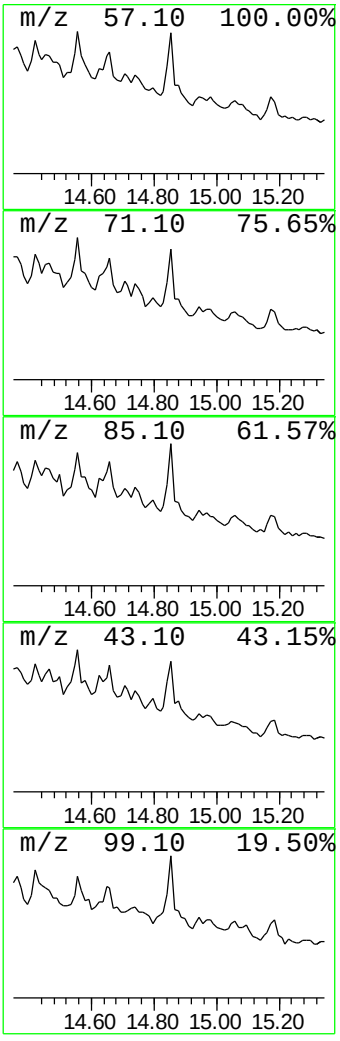
Peak Number 14 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.71 ng	121768	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Nonacosane	408	C29H60	000630-03-5	86
4	Pentacosane	352	C25H52	000629-99-2	83
5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : WQ-5W

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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
2-Pentanone, 4-hy...	4.74	11.1	ng	602875	1	6.61	1086430	20.0
unknown6.38	6.38	57.9	ng	3147510	1	6.61	1086430	20.0
Hexanoic acid, 2-...	7.37	8.3	ng	613040	2	7.90	1469680	20.0
Triacetin	8.70	7.8	ng	572088	2	7.90	1469680	20.0
3,6,9,12-Tetraoxa...	10.78	5.0	ng	451429	4	11.14	1816040	20.0
Eicosane	11.02	4.3	ng	386886	4	11.14	1816040	20.0
Dodecane	12.61	2.1	ng	136995	5	13.77	1301310	20.0
Hexadecane	13.09	2.3	ng	149700	5	13.77	1301310	20.0
unknown13.31	13.31	3.0	ng	196157	5	13.77	1301310	20.0
Octadecane, 1-chl...	13.64	5.1	ng	332760	5	13.77	1301310	20.0
Pentadecane	14.26	4.5	ng	293280	5	13.77	1301310	20.0
unknown14.56	14.56	3.1	ng	140967	6	15.14	897823	20.0
Heneicosane	14.85	2.7	ng	121768	6	15.14	897823	20.0