LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

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-BF102616.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	4.556	213	216	225	rBV	50603	79240	1.20%	0.135%
2	4.887	242	245	256	rBV	694193	1224114	18.51%	2.078%
3	5.321	280	283	286	rBV	3955890	4827645	73.02%	8.195%
4	5.653	311	312	322	rBV	62164	100804	1.52%	0.171%
5	5.961	336	339	340	rBV	232306	271607	4.11%	0.461%
6	5.996	340	342	353	rVB	594247	757959	11.46%	1.287%
7	6.373	372	375	383	rBV	3988063	6112721	92.45%	10.377%
8	6.499	383	386	388	rVB	4210078	6258345	94.66%	10.624%
9	6.716	403	405	408	rBV	1013946	1125102	17.02%	1.910%
10	6.876	416	419	433	rBV2	4484467	6397258	96.76%	10.860%
11	7.287	452	455	458	rBV	2482447	3845065	58.16%	6.527%
12	7.413	462	466	469	rVB	70040	135844	2.05%	0.231%
13	8.007	516	518	526	rBV	1716330	1641520	24.83%	2.787%
14	9.093	609	613	615	rBV	6355436	6611682	100.00%	11.224%
15	9.493	645	648	650	rBV	1327949	1773379	26.82%	3.010%
16	9.756	669	671	673	rVV	1198926	1558673	23.57%	2.646%
17	9.790	673	674	677	rVB	96781	87518	1.32%	0.149%
18	9.962	688	689	693	rBV2	40746	68912	1.04%	0.117%
19	10.202	709	710	712	rVB	148730	118516	1.79%	0.201%
20	10.305	718	719	723	rVB	92354	91827	1.39%	0.156%
21	10.419	726	729	732	rBV2	51050	82645	1.25%	0.140%
22	10.556	738	741	743	rBV	3460893	3879338	58.67%	6.586%
23	10.670	750	751	755	rBV	139837	217056	3.28%	0.368%
24	11.128	789	791	796	rVB2	80277	166543	2.52%	0.283%
25	11.242	799	801	802	rBV	1535591	1367385	20.68%	2.321%
26	11.322	805	808	810	rVB	124429	186557	2.82%	0.317%
27	11.482	819	822	826	rBV2	106558	150865	2.28%	0.256%
28	11.859	853	855	860	rVB2	75992	138644	2.10%	0.235%
29	12.454	904	907	909	rBV	616751	593143	8.97%	1.007%
30	12.682	923	927	929	rBV	352275	546356	8.26%	0.927%
31	12.831	937	940	943	rBV	4335346	4433312	67.05%	7.526%
32	13.014	951	956	957	rBV	68412	93139	1.41%	0.158%
33	13.071	960	961	963	rVB	61333	72685	1.10%	0.123%
34	13.734	1017	1019	1023	rBV	439184	499516	7.56%	0.848%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.871	1028	1031	1038	rVB2	886021	1390727	21.03%	2.361%
36	13.985	1038	1041	1042	rBV	45891	66621	1.01%	0.113%
37	14.362	1071	1074	1080	rBV4	47524	140717	2.13%	0.239%
38	14.579	1090	1093	1096	rBV2	36172	83311	1.26%	0.141%
39	14.877	1117	1119	1124	rBV	135675	305608	4.62%	0.519%
40	15.151	1141	1143	1146	rBV	67296	98581	1.49%	0.167%
41	15.208	1146	1148	1151	rVB	106698	159572	2.41%	0.271%
42	15.277	1151	1154	1156	rBV	574985	868807	13.14%	1.475%
43	15.745	1193	1195	1200	rBV2	54128	99773	1.51%	0.169%
44	16.591	1266	1269	1274	rVB2	49131	104741	1.58%	0.178%
45	16.991	1300	1304	1308	rBV	30484	73750	1.12%	0.125%

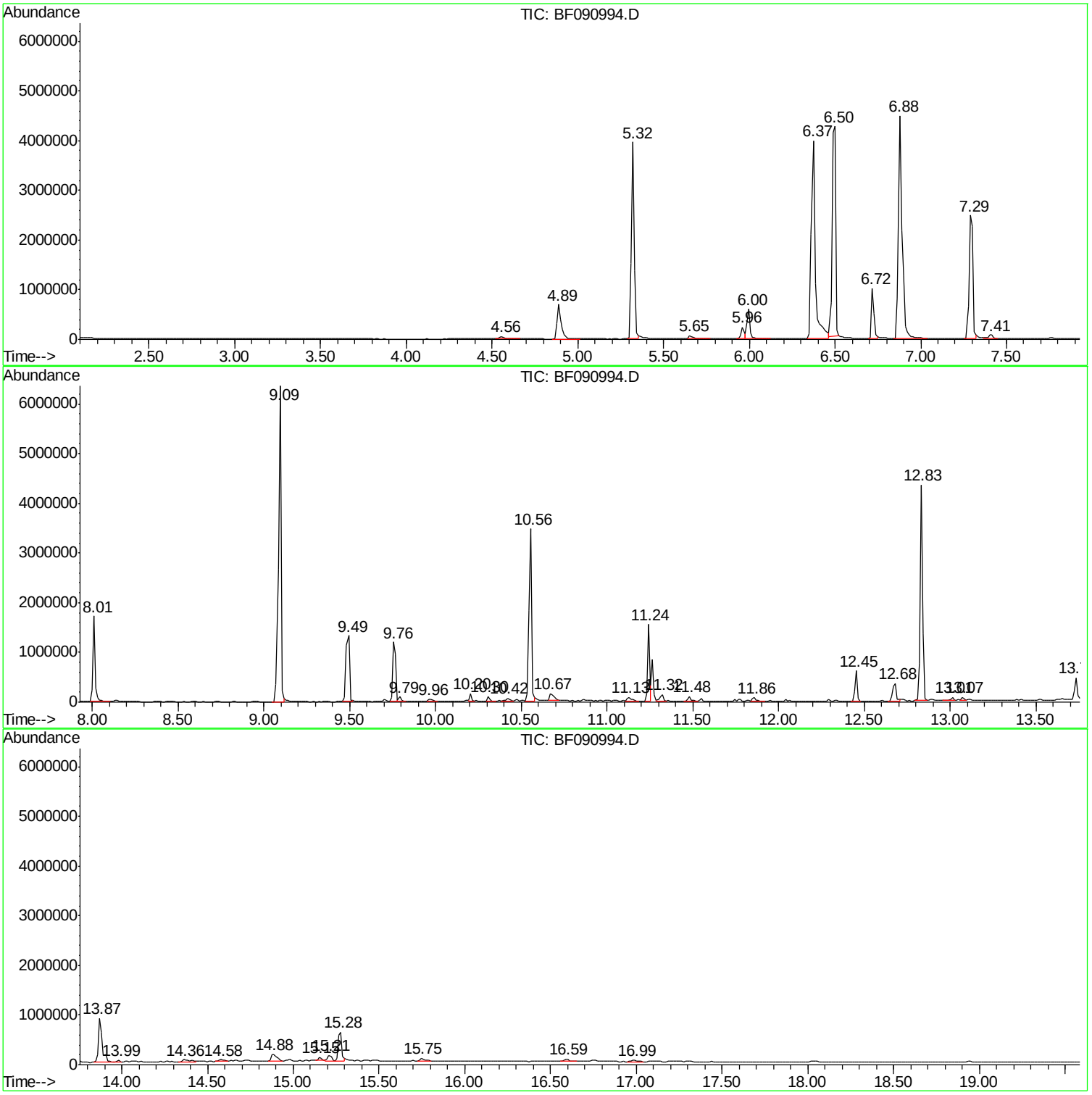
Sum of corrected areas: 58907123

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

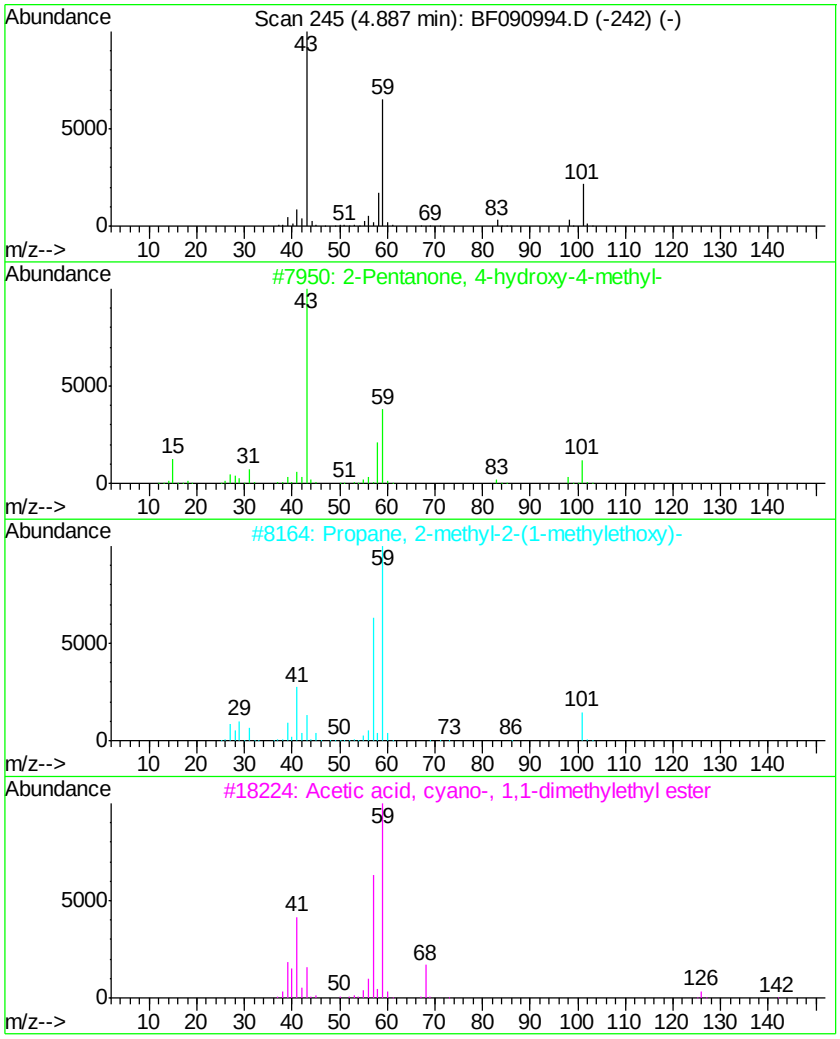
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

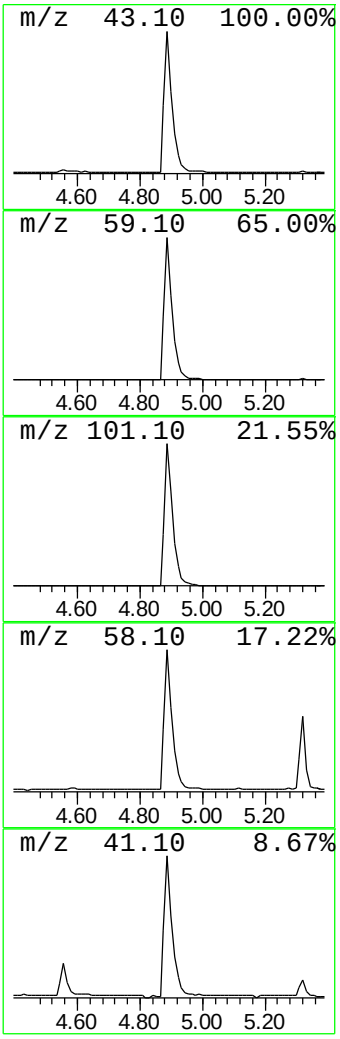
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	21.76 ng	1224110	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

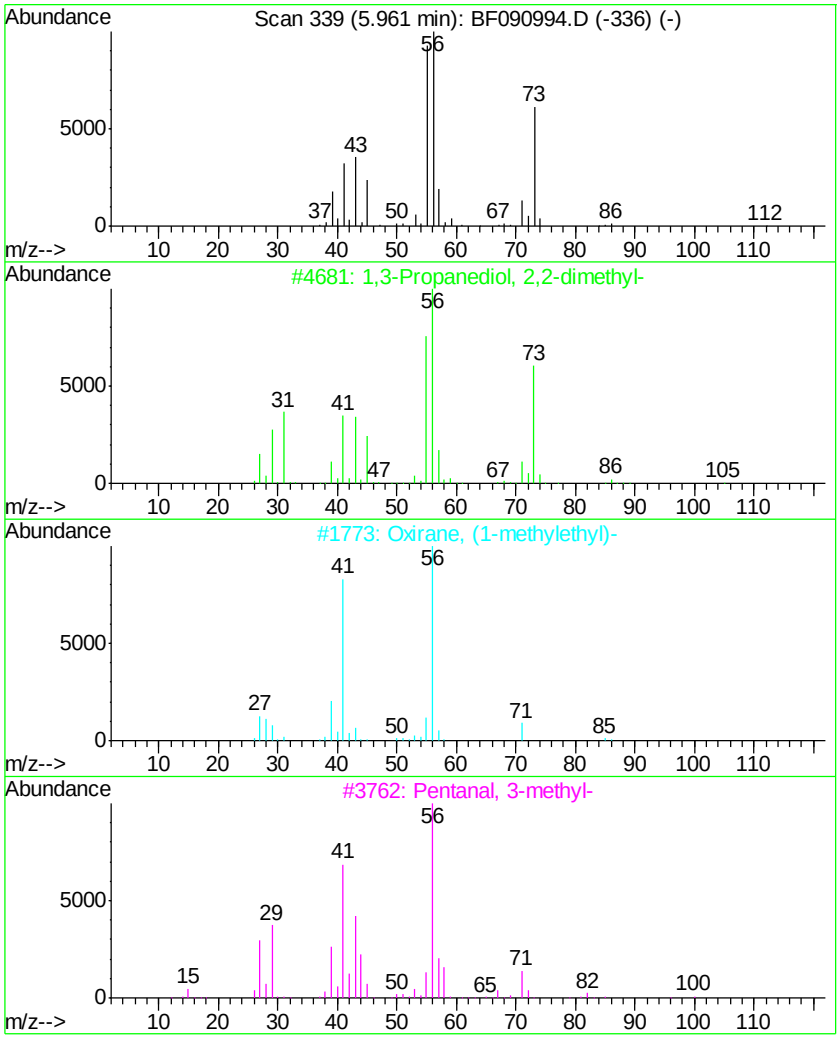
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

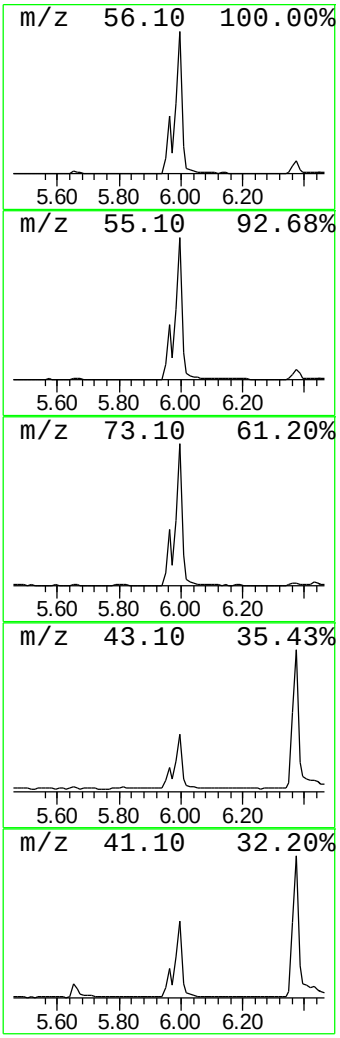
****

Peak Number 2 1,3-Propanediol, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	4.83 ng	271607	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Propanediol, 2,2-dimethyl-	104	C5H12O2	000126-30-7	83
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	49
3	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	40
4	4-Heptanol	116	C7H16O	000589-55-9	12
5	1-Hepten-4-ol	114	C7H14O	003521-91-3	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

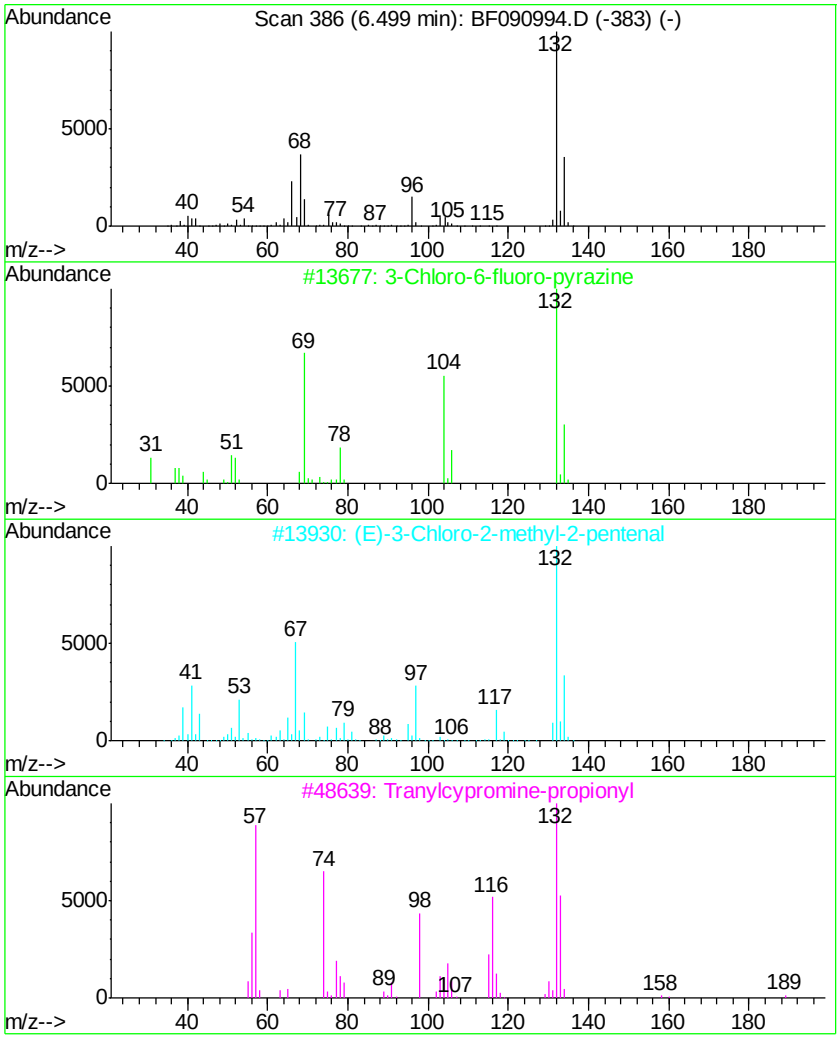
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

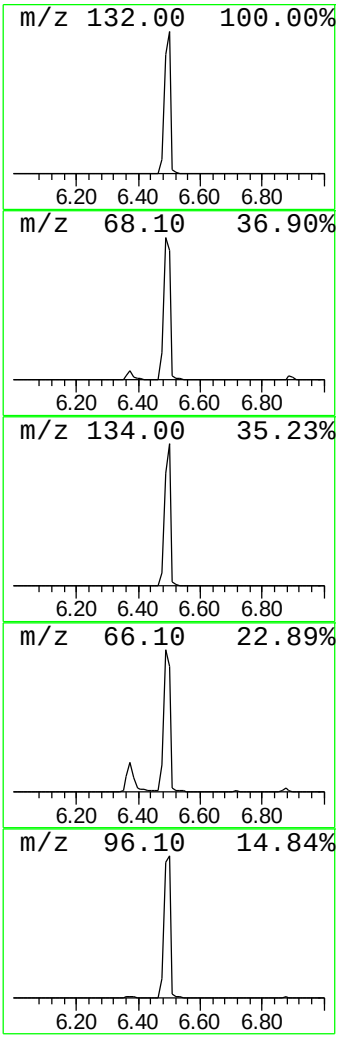
****

Peak Number 4 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	111.25 ng	6258350	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

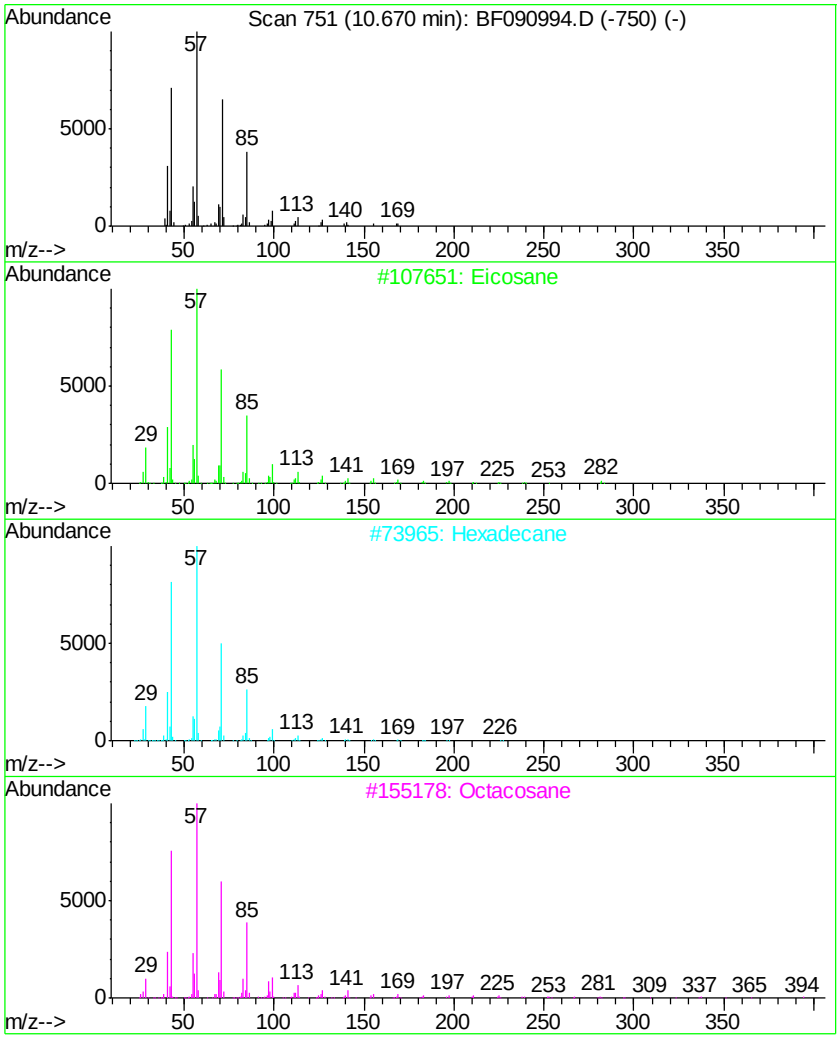
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

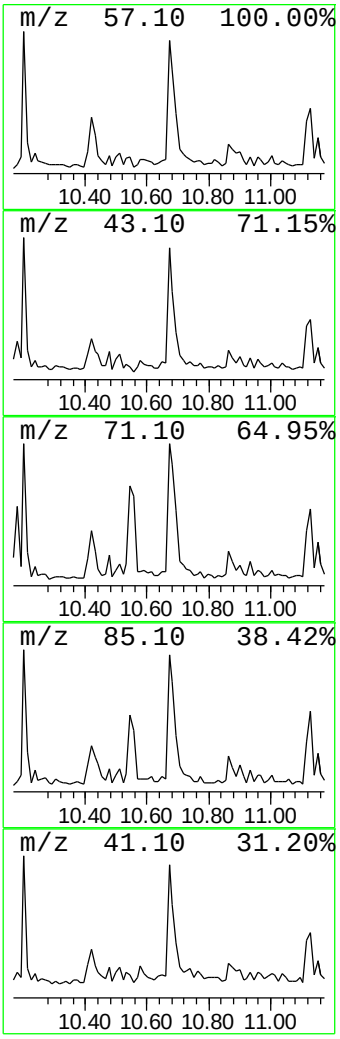
****

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.17 ng	217056	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Hexadecane	226	C16H34	000544-76-3	80
3	Octacosane	394	C28H58	000630-02-4	78
4	Pentadecane	212	C15H32	000629-62-9	78
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

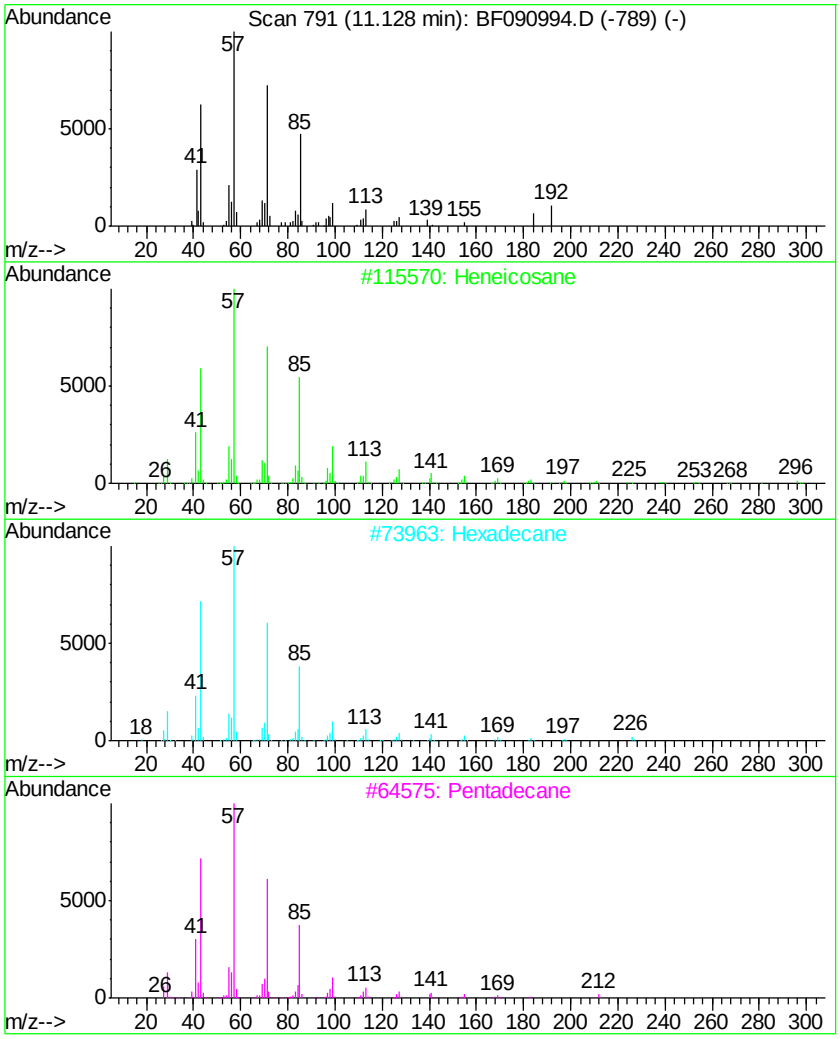
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

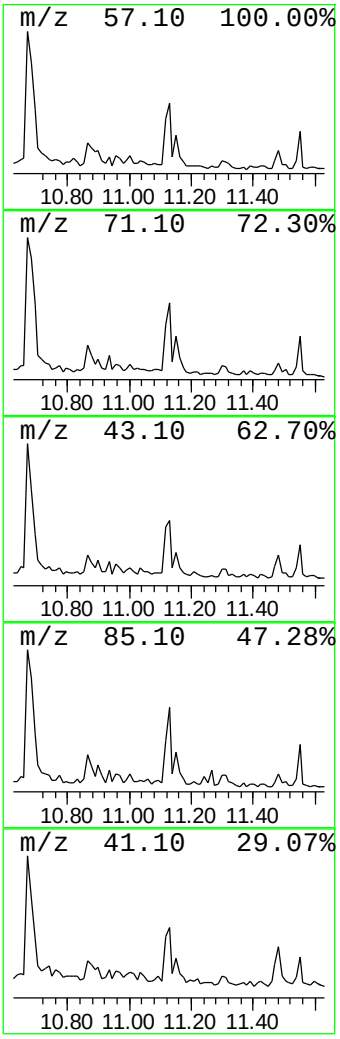
****

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	2.44 ng	166543	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Hexadecane	226	C16H34	000544-76-3	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

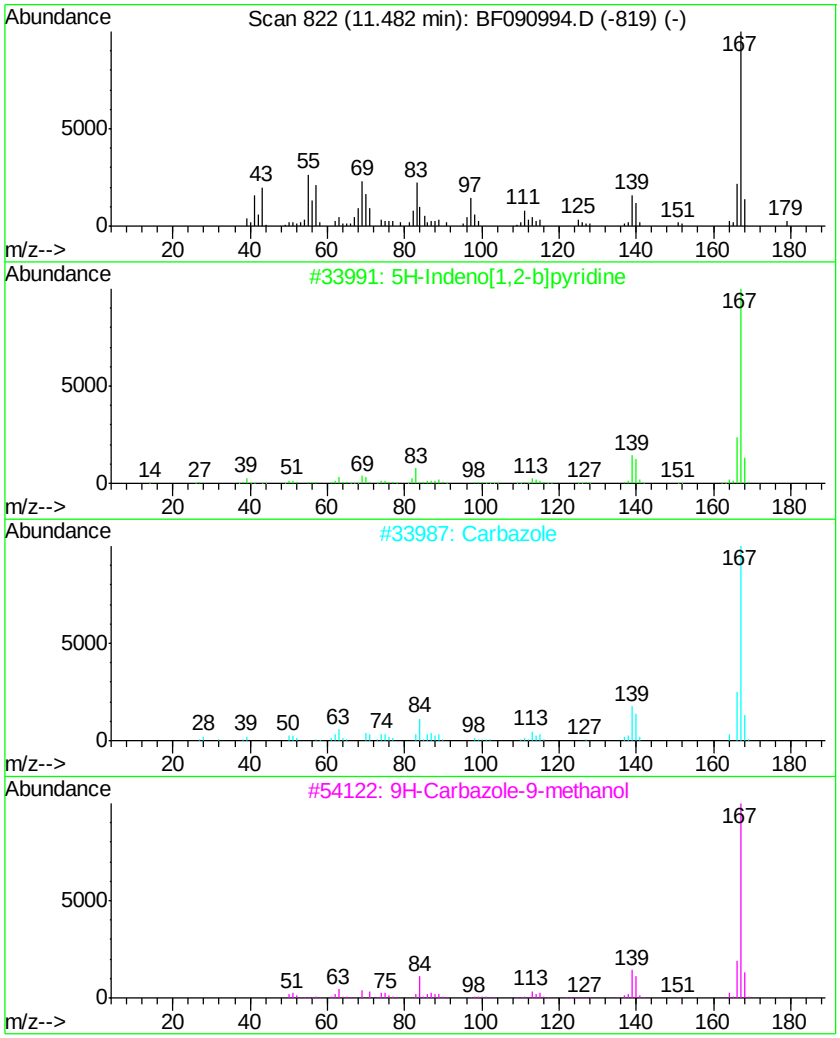
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

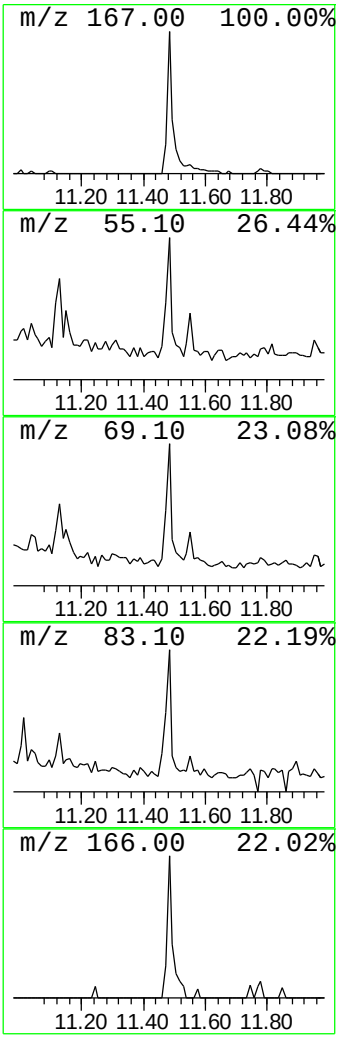
****

Peak Number 8 5H-Indeno[1,2-b]pyridine Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.48	2.21 ng	150865	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	94
2	Carbazole	167	C12H9N	000086-74-8	94
3	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	74
4	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	64
5	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

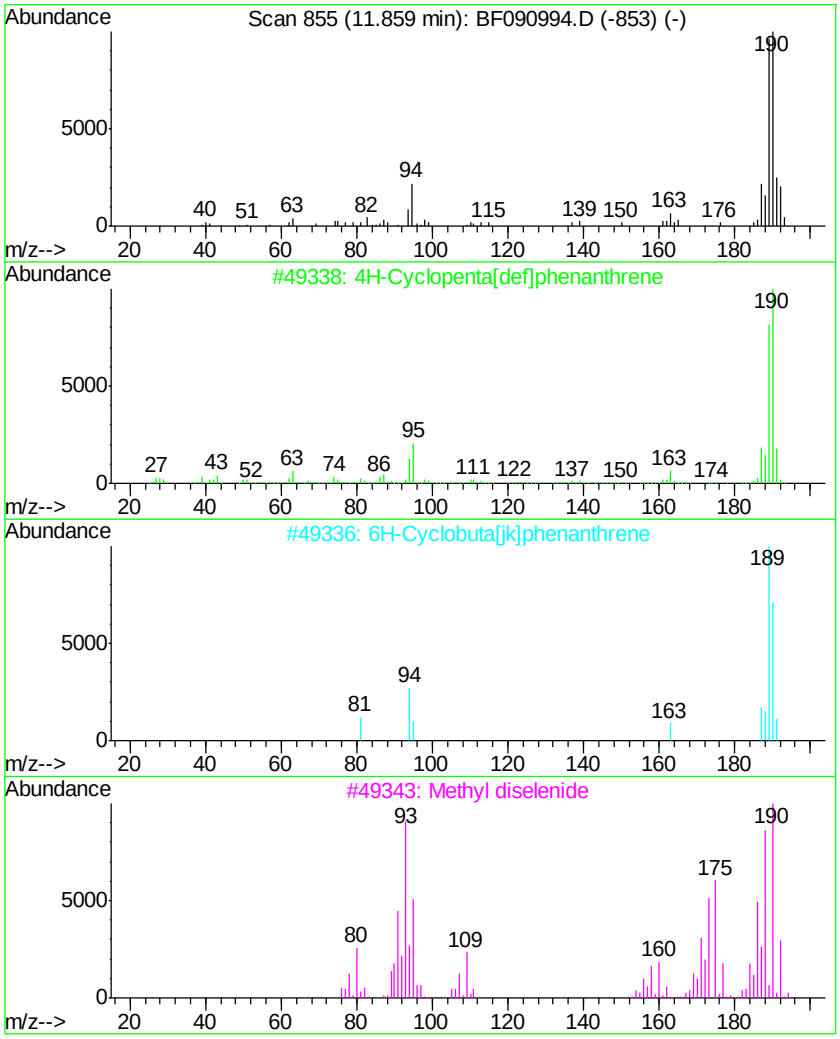
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

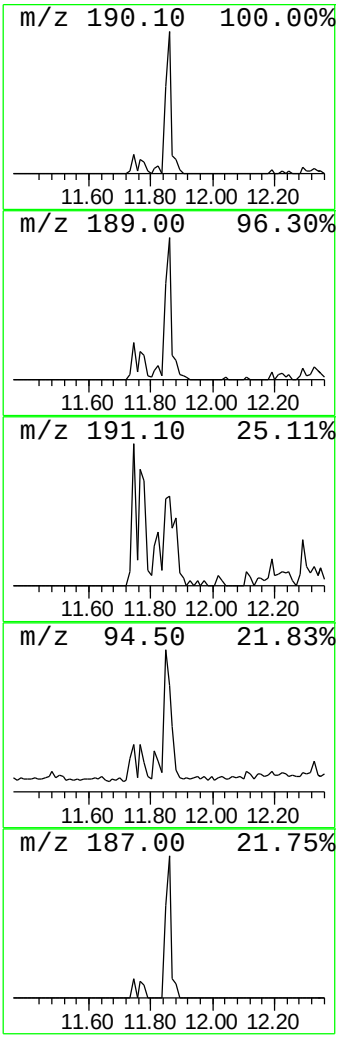
****

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.03 ng	138644	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	55
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

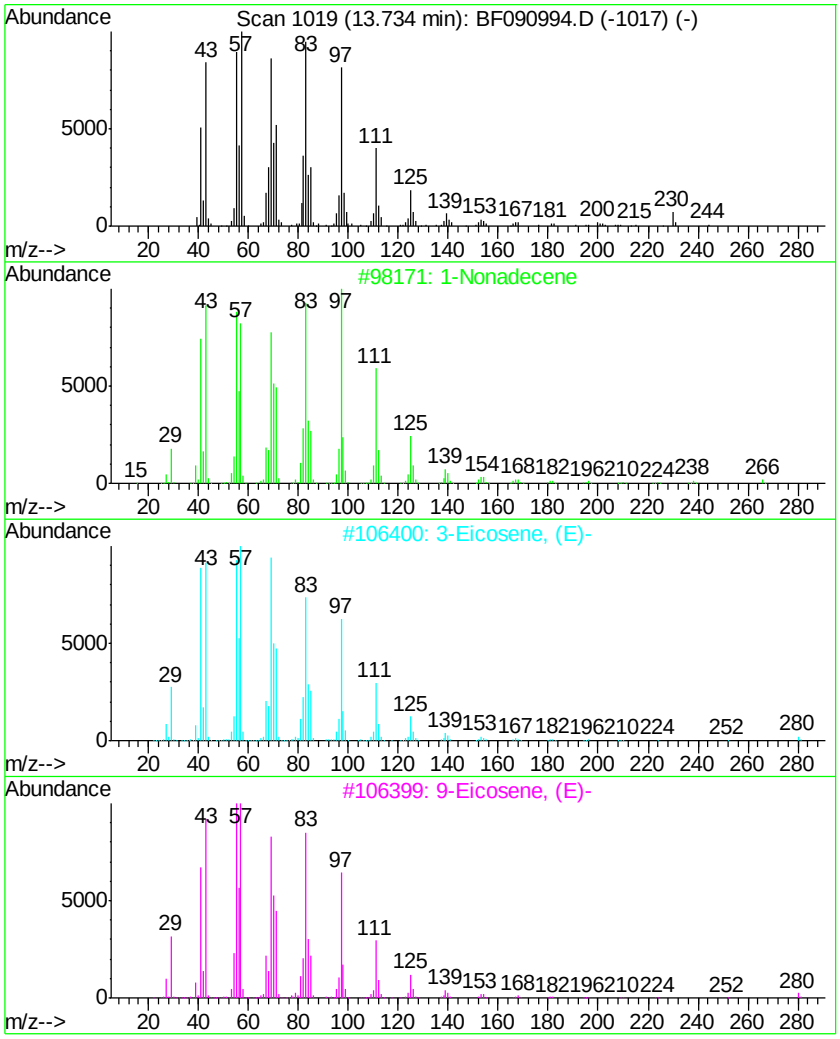
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

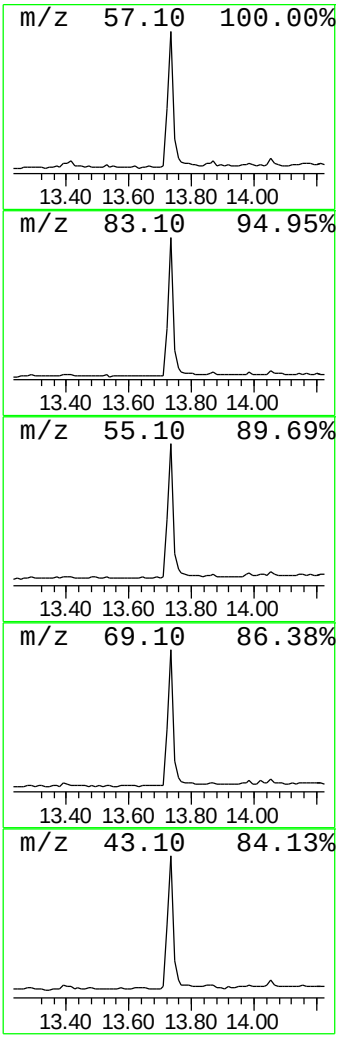
****

Peak Number 10 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.18 ng	499516	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

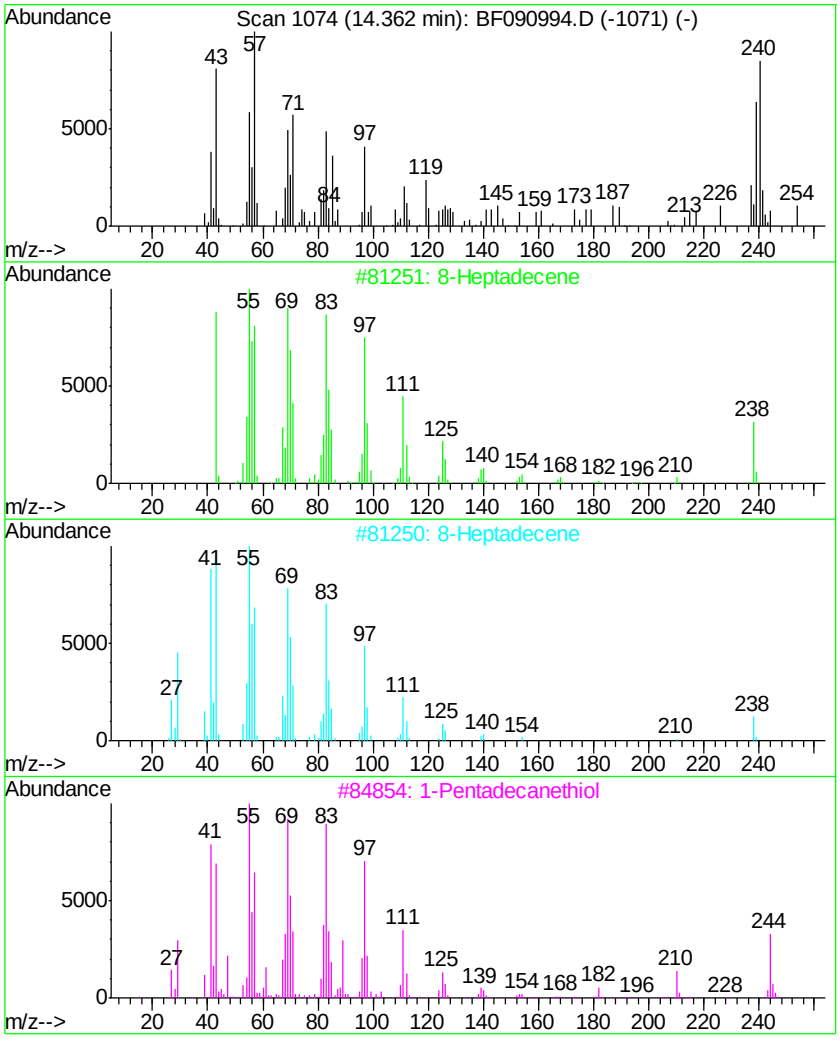
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

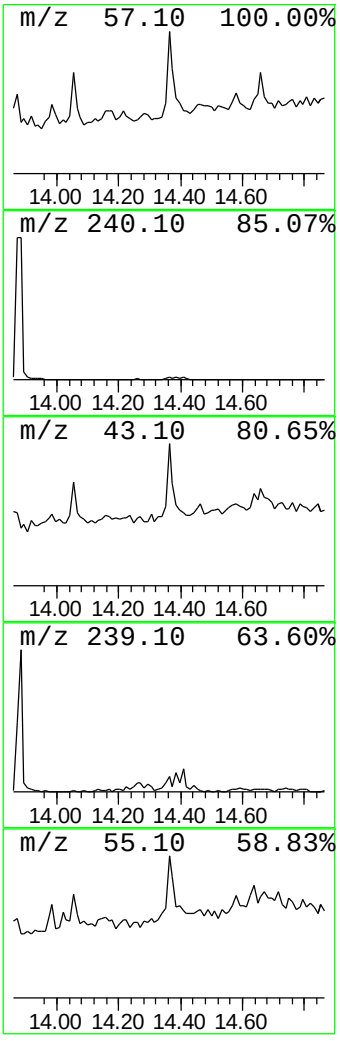
****

Peak Number 11 unknown14.36 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.02 ng	140717	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Heptadecene	238	C17H34	002579-04-6	42
2	8-Heptadecene	238	C17H34	054290-12-9	38
3	1-Pentadecanethiol	244	C15H32S	025276-70-4	38
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	30
5	3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	30





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

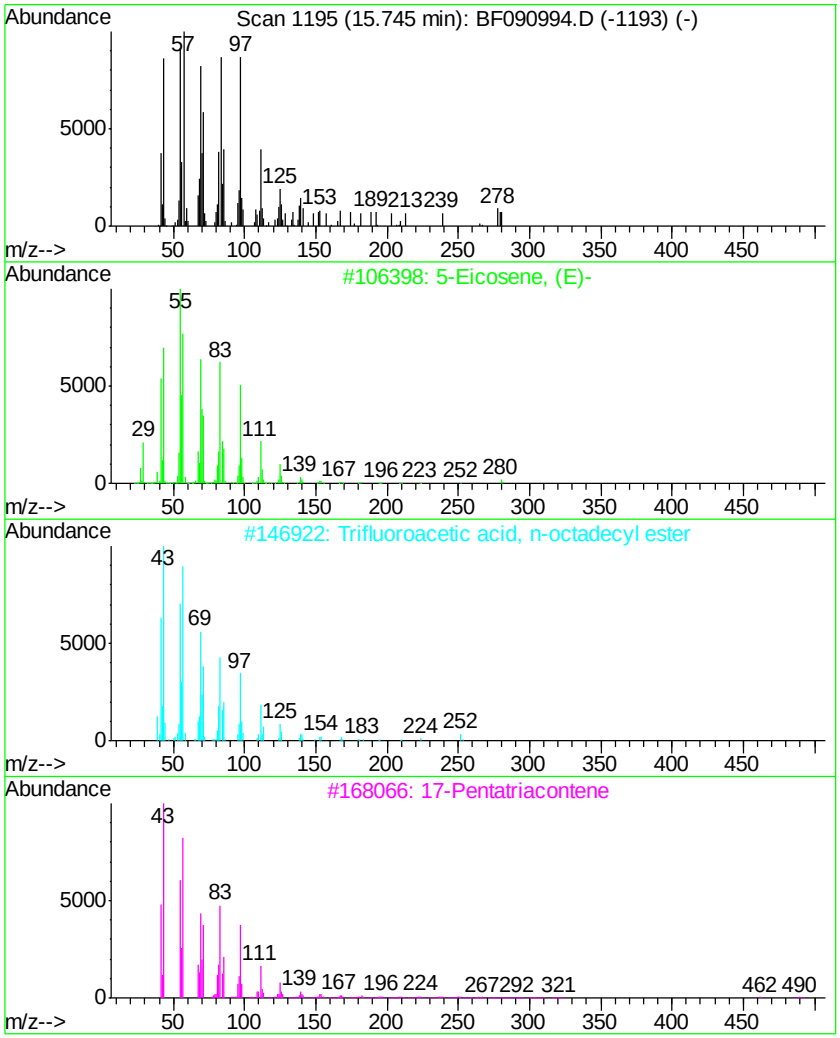
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

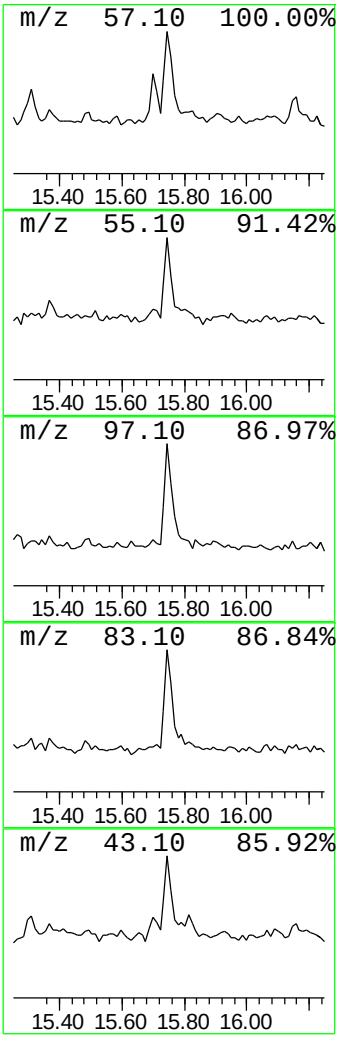
****

Peak Number 13 5-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.30 ng	99773	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	86
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	86
3	17-Pentatriacontene	491	C35H70	006971-40-0	83
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090994.D
Acq On : 2 Nov 2016 21:51
Operator : UM/SJ
Sample : H5509-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-1-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.89	21.8	ng	1224110	1	6.72	1125100	20.0
1,3-Propanediol, ...	5.96	4.8	ng	271607	1	6.72	1125100	20.0
unknown6.50	6.50	111.3	ng	6258350	1	6.72	1125100	20.0
Eicosane	10.67	3.2	ng	217056	4	11.24	1367390	20.0
Heneicosane	11.13	2.4	ng	166543	4	11.24	1367390	20.0
5H-Indeno[1,2-b]p...	11.48	2.2	ng	150865	4	11.24	1367390	20.0
4H-Cyclopenta[def...	11.86	2.0	ng	138644	4	11.24	1367390	20.0
1-Nonadecene	13.73	7.2	ng	499516	5	13.87	1390730	20.0
unknown14.36	14.36	2.0	ng	140717	5	13.87	1390730	20.0
5-Eicosene, (E)-	15.75	2.3	ng	99773	6	15.28	868807	20.0