LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

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-BF092815.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	5.040	251	254	264	rVB	693013	1003135	50.19%	4.227%
2	5.451	288	290	293	rBV	1727837	1847544	92.43%	7.785%
3	6.492	378	381	383	rBV	1629680	1998847	100.00%	8.422%
4	6.617	390	392	395	rBV	2067707	1973309	98.72%	8.314%
5	6.846	410	412	415	rBV	604524	603350	30.18%	2.542%
6	7.006	423	426	428	rBV	1754635	1592000	79.65%	6.708%
7	7.417	460	462	465	rBV	1059981	1118959	55.98%	4.715%
8	7.509	468	470	476	rVB	17174	33618	1.68%	0.142%
9	8.035	515	516	518	rBV	13946	20076	1.00%	0.085%
10	8.137	522	525	527	rBV	885337	797190	39.88%	3.359%
11	9.086	606	608	610	rVB	37906	34845	1.74%	0.147%
12	9.212	617	619	622	rBV	1577421	1797638	89.93%	7.574%
13	9.555	644	649	651	rBV3	8726	20303	1.02%	0.086%
14	9.612	652	654	656	rVV	410040	336875	16.85%	1.419%
15	9.749	665	666	669	rBV2	17976	30065	1.50%	0.127%
16	9.818	669	672	674	rBV2	16198	26199	1.31%	0.110%
17	9.898	676	679	681	rBV	743313	813439	40.70%	3.427%
18	10.092	694	696	699	rBV2	14439	21856	1.09%	0.092%
19	10.298	712	714	715	rBV	33853	41627	2.08%	0.175%
20	10.321	715	716	717	rVB	47964	33498	1.68%	0.141%
21	10.435	724	726	729	rVB	22478	30345	1.52%	0.128%
22	10.538	733	735	738	rVB	29302	41111	2.06%	0.173%
23	10.686	745	748	750	rBV	1061630	1128923	56.48%	4.757%
24	10.801	756	758	762	rVB	75974	124900	6.25%	0.526%
25	10.983	772	774	776	rBV3	13886	24187	1.21%	0.102%
26	11.132	783	787	788	rBV3	12411	28175	1.41%	0.119%
27	11.246	794	797	798	rBV2	38719	66065	3.31%	0.278%
28	11.269	798	799	802	rVB2	52798	54769	2.74%	0.231%
29	11.338	802	805	807	rBV2	16644	25373	1.27%	0.107%
30	11.383	807	809	814	rBV2	609714	897380	44.89%	3.781%
31	11.452	814	815	817	rVB	52010	46338	2.32%	0.195%
32	11.624	825	830	832	rBV5	20066	59181	2.96%	0.249%
33	11.669	832	834	836	rVB	43591	39788	1.99%	0.168%
34	11.909	853	855	857	rBV	250766	220434	11.03%	0.929%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

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-BF092815.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.944	857	858	861	rVB2	19386	25799	1.29%	0.109%
36	11.989	861	862	868	rVB	64051	105201	5.26%	0.443%
37	12.069	868	869	872	rBV	26915	35355	1.77%	0.149%
38	12.184	875	879	882	rBV3	18178	48442	2.42%	0.204%
39	12.424	898	900	902	rBV	28546	36959	1.85%	0.156%
40	12.469	902	904	905	rVB	22575	26736	1.34%	0.113%
41	12.595	912	915	917	rBV	396094	396598	19.84%	1.671%
42	12.629	917	918	921	rVB3	19893	21780	1.09%	0.092%
43	12.686	921	923	927	rBV3	35355	68399	3.42%	0.288%
44	12.789	930	932	933	rBV	223299	281748	14.10%	1.187%
45	12.824	933	935	937	rVB	296388	306180	15.32%	1.290%
46	12.972	945	948	950	rBV	1024520	1290685	64.57%	5.438%
47	13.052	952	955	958	rVB3	41475	74769	3.74%	0.315%
48	13.098	958	959	960	rBV	25896	22390	1.12%	0.094%
49	13.155	962	964	966	rVV	31324	47577	2.38%	0.200%
50	13.212	966	969	971	rVV2	25864	49794	2.49%	0.210%
51	13.258	971	973	976	rVB3	28724	44917	2.25%	0.189%
52	13.487	991	993	995	rBV2	121855	161233	8.07%	0.679%
53	13.532	995	997	1002	rVV3	37978	75916	3.80%	0.320%
54	13.829	1021	1023	1024	rBV	44981	68178	3.41%	0.287%
55	13.864	1024	1026	1032	rVB2	222451	345940	17.31%	1.458%
56	14.001	1036	1038	1046	rBV3	746222	1687283	84.41%	7.109%
57	14.127	1047	1049	1050	rVV2	33659	31071	1.55%	0.131%
58	14.184	1052	1054	1056	rVB3	69222	87522	4.38%	0.369%
59	14.492	1078	1081	1083	rBV3	69359	118503	5.93%	0.499%
60	14.790	1105	1107	1108	rBV	51317	60684	3.04%	0.256%
61	15.052	1127	1130	1134	rBV	122836	269755	13.50%	1.137%
62	15.338	1153	1155	1158	rVB	66743	82958	4.15%	0.350%
63	15.407	1158	1161	1164	rVV	88698	155736	7.79%	0.656%
64	15.464	1164	1166	1172	rVB	347754	534279	26.73%	2.251%
65	15.955	1206	1209	1213	rVB4	37780	82498	4.13%	0.348%
66	16.881	1287	1290	1294	rBV2	37892	76053	3.80%	0.320%
67	17.304	1324	1327	1333	rVB	35551	81184	4.06%	0.342%

Sum of corrected areas: 23733464

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
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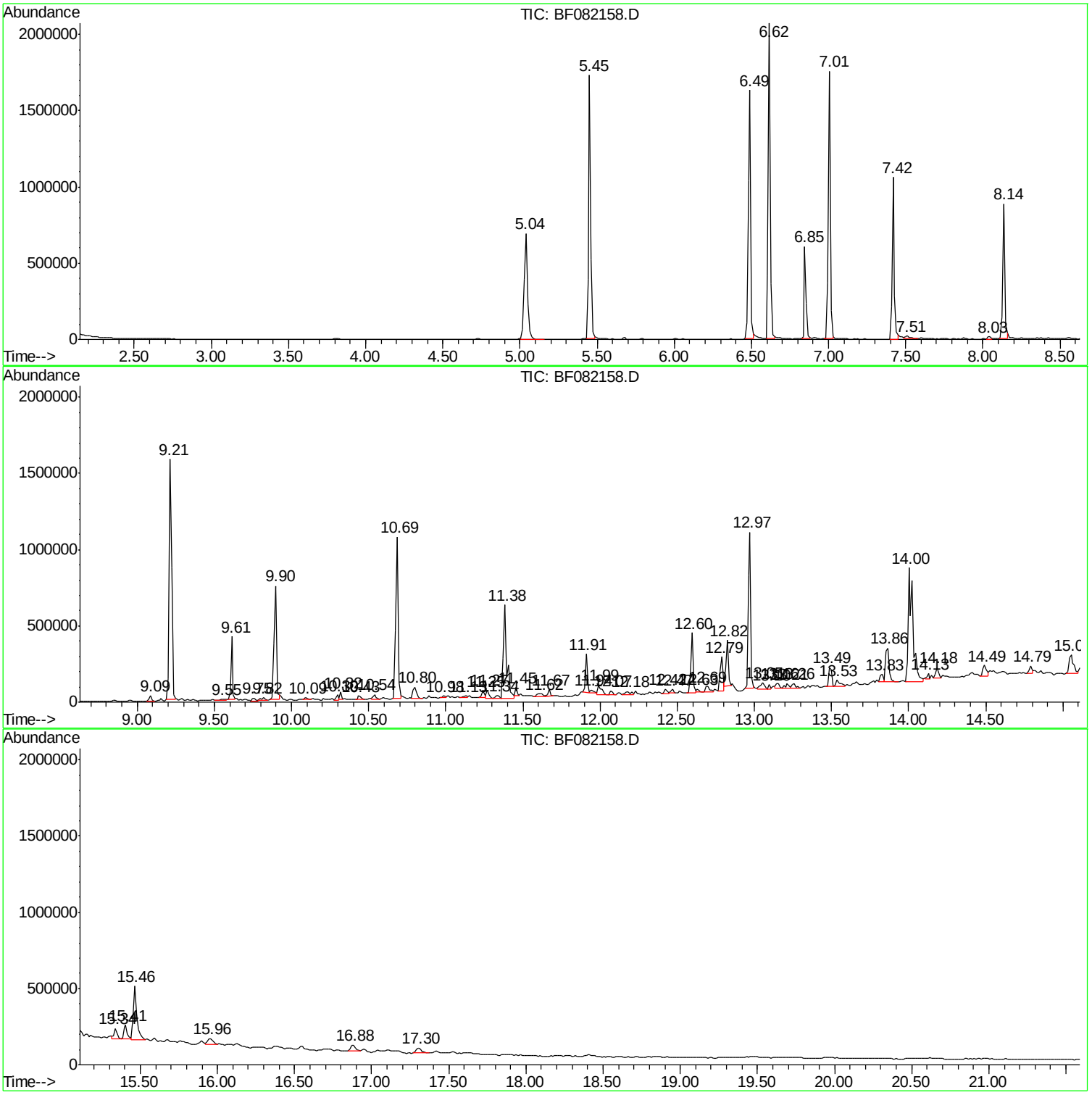
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

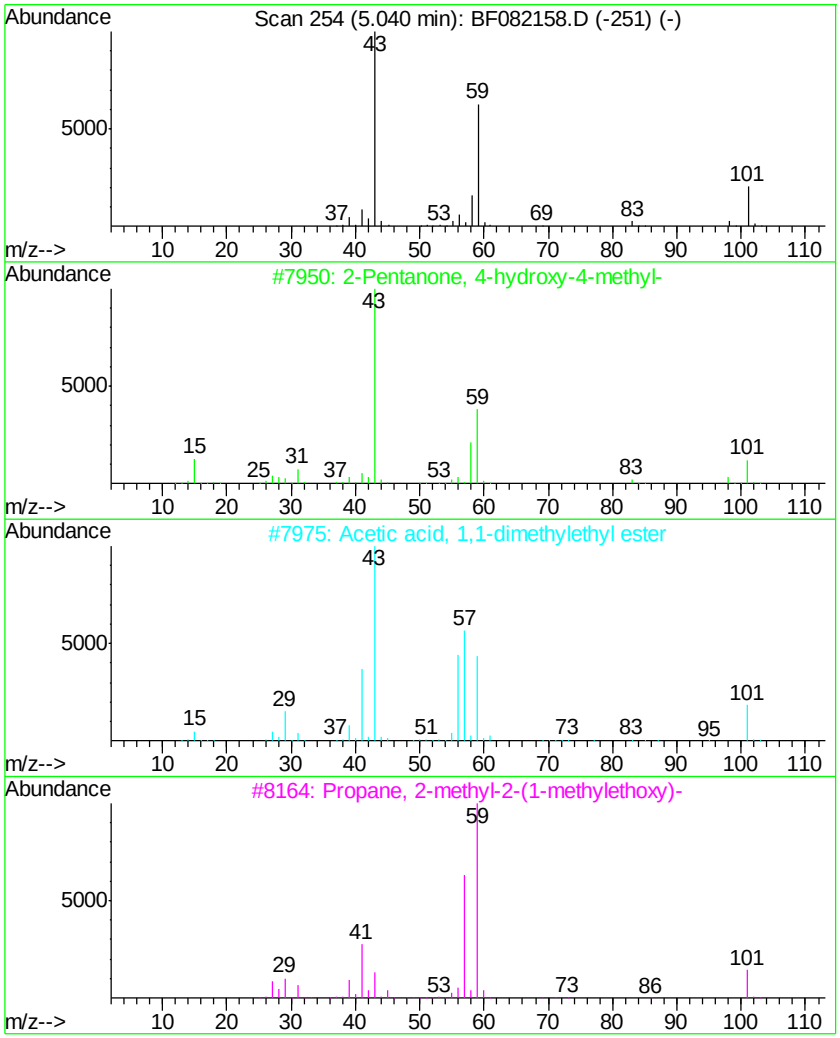
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

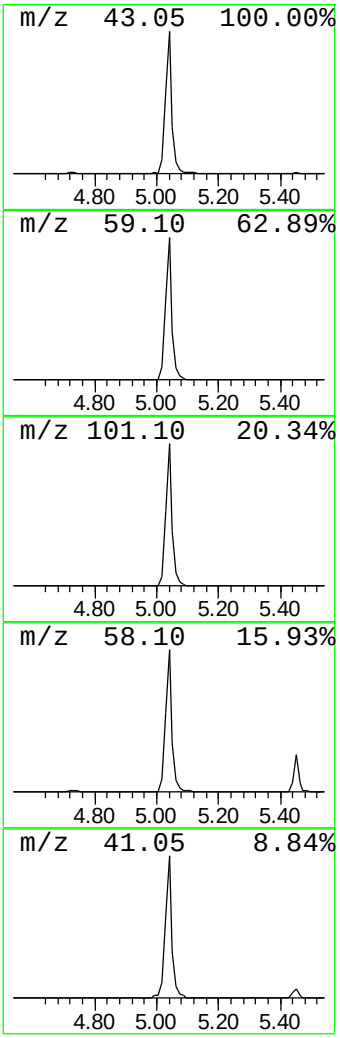
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	33.25 ng	1003140	1,4-Dichlorobenzene-d4	6.85

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	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

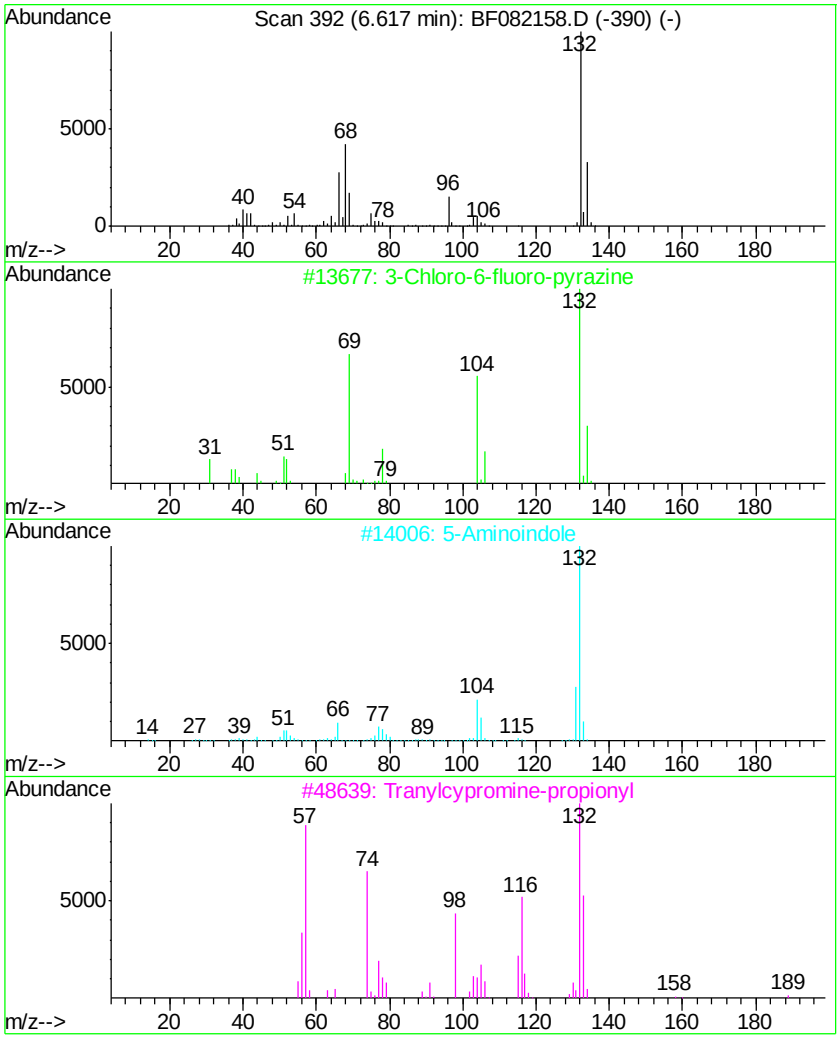
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

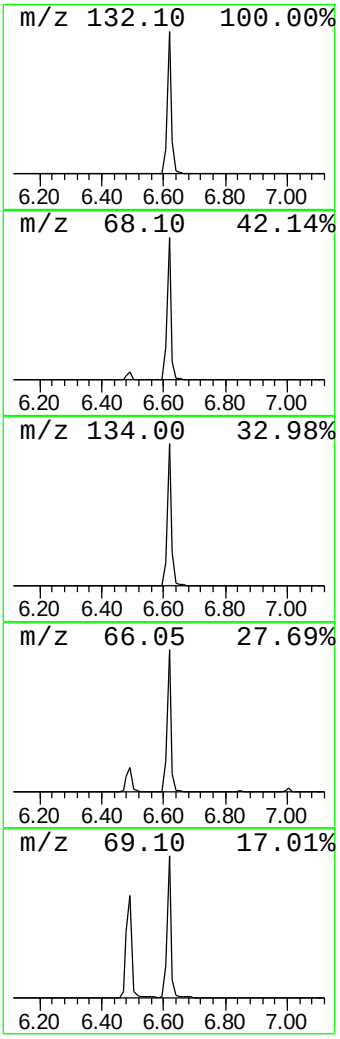
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	65.41 ng	1973310	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF082158.D
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Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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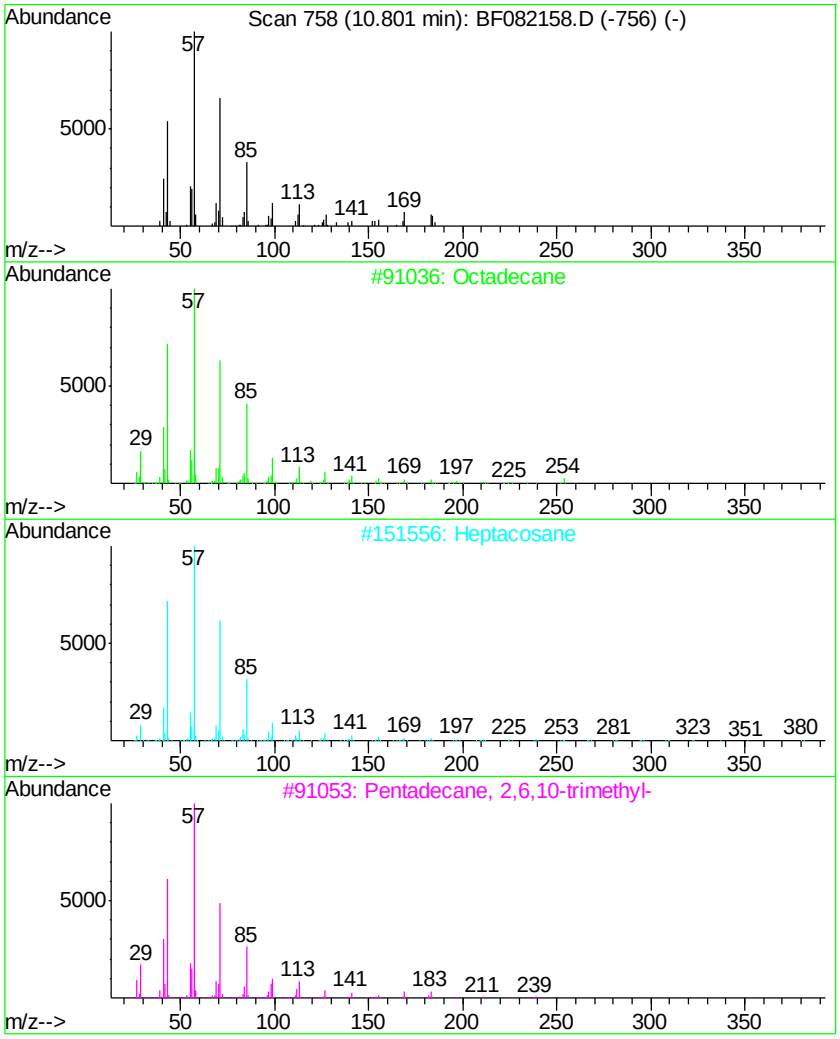
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

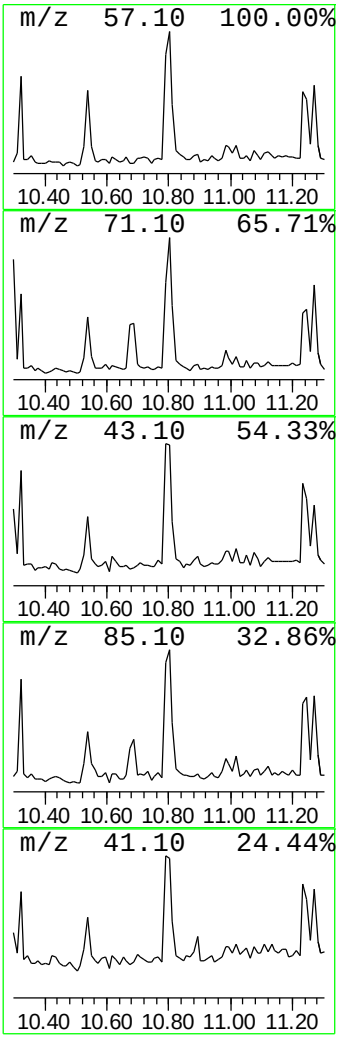
****

Peak Number 4 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.78 ng	124900	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Heptacosane	380	C27H56	000593-49-7	86
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Tridecane	184	C13H28	000629-50-5	81





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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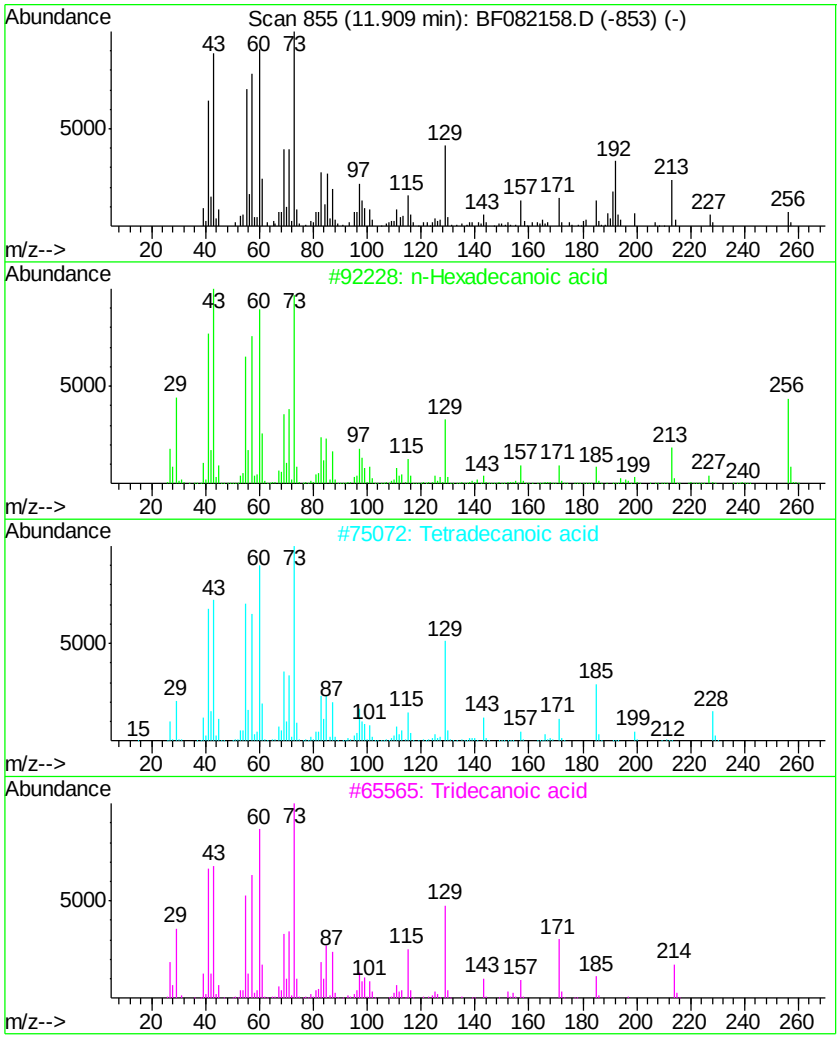
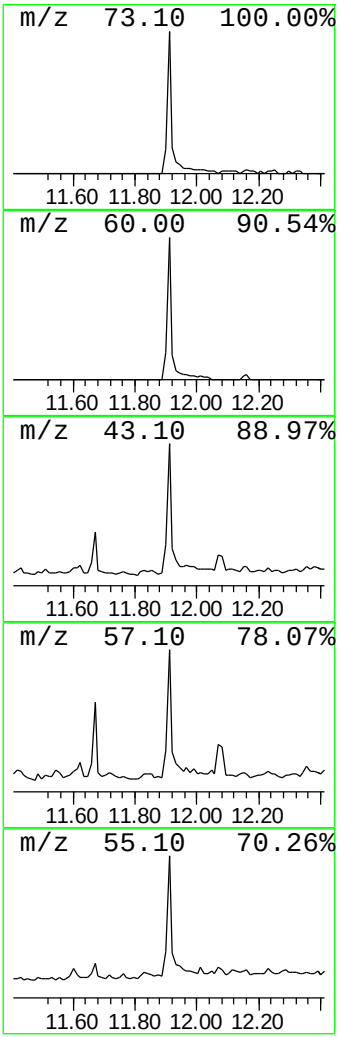
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	4.91 ng	220434	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	20





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Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

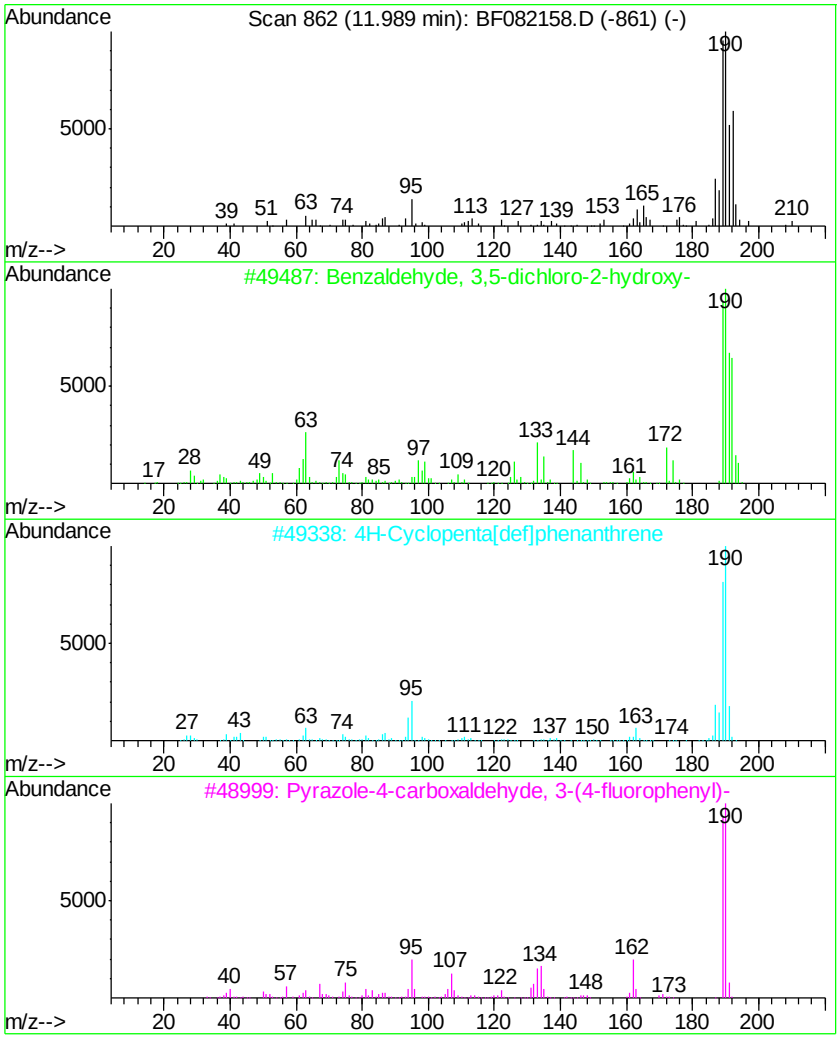
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

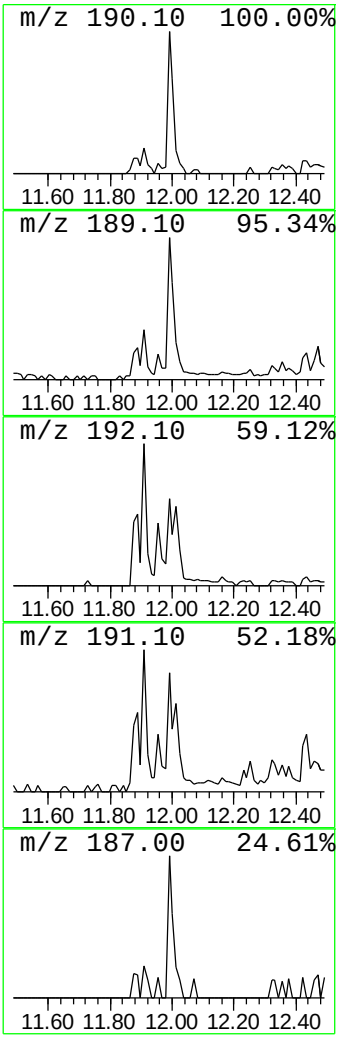
****

Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.34 ng	105201	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	46
4	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	25
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
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Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

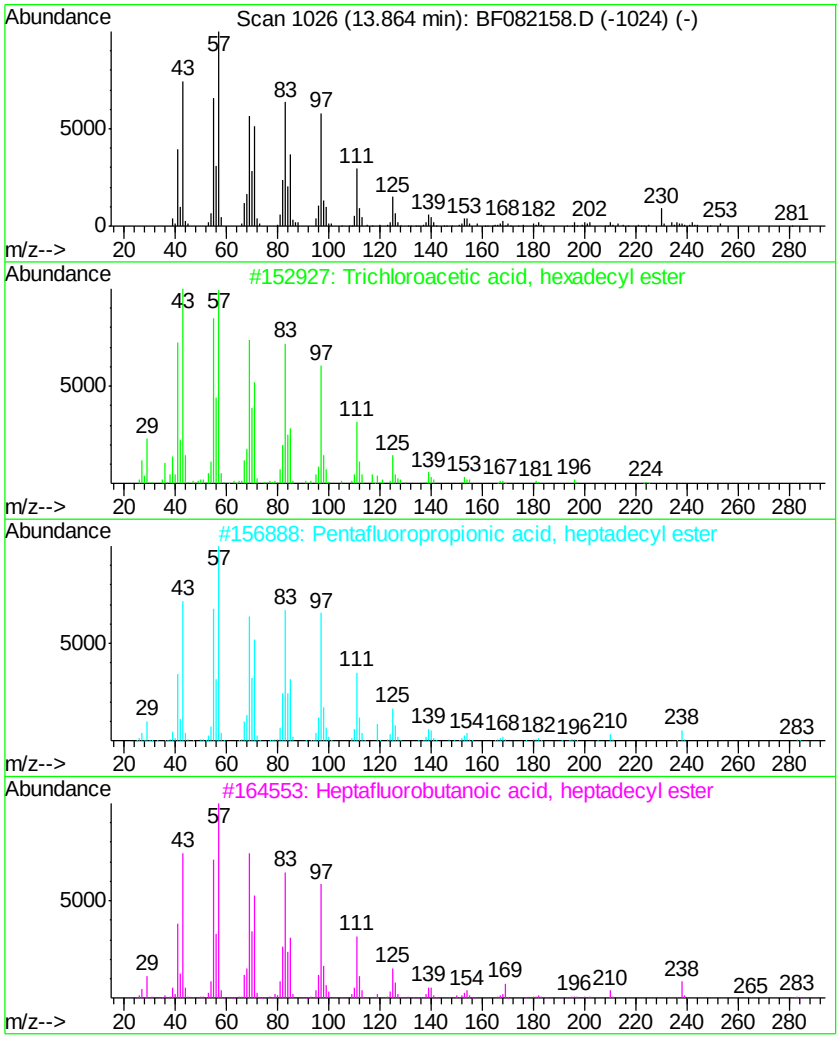
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

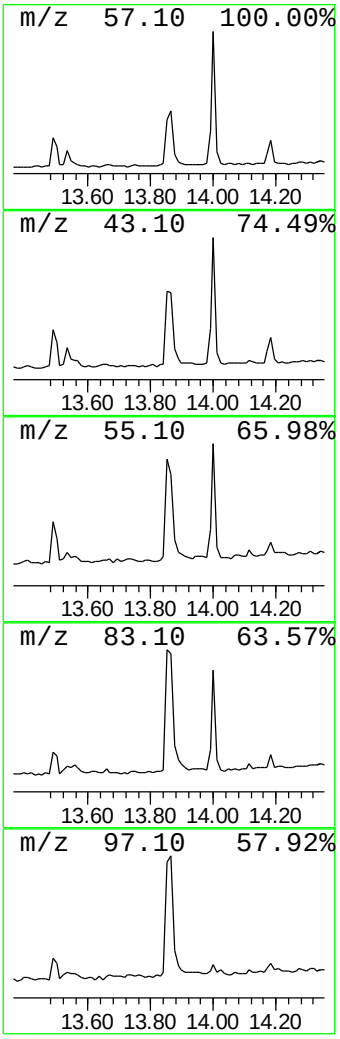
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.10 ng	345940	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

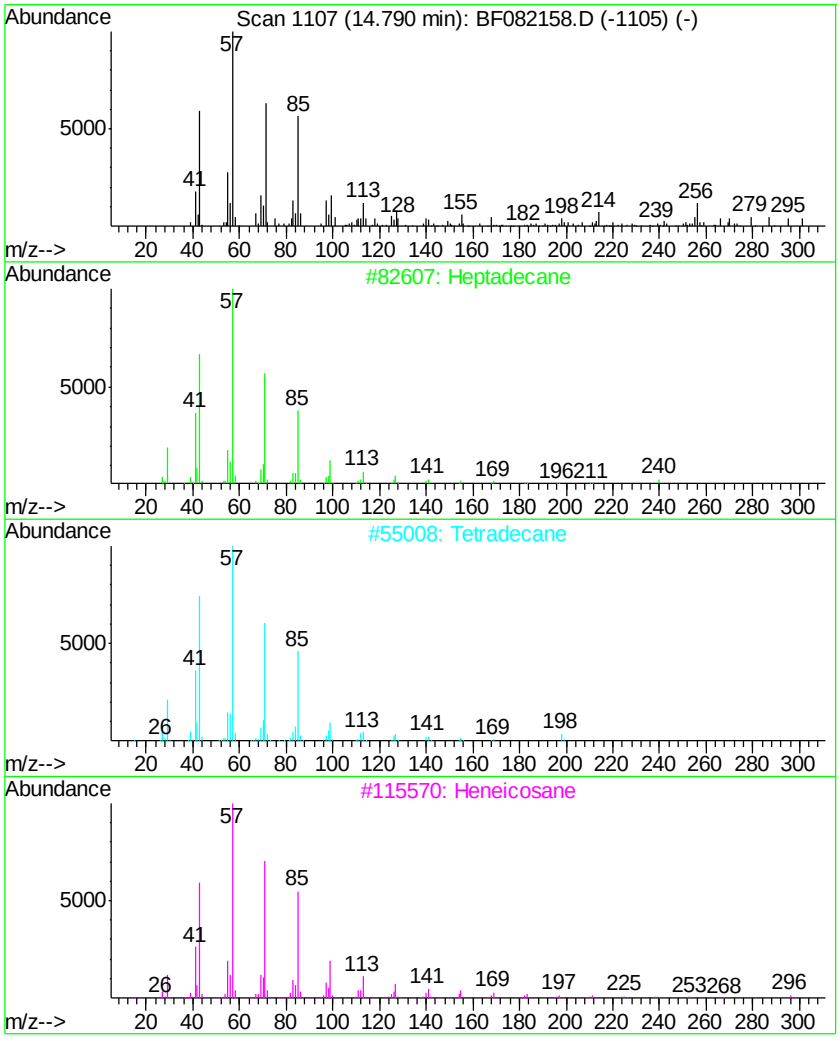
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

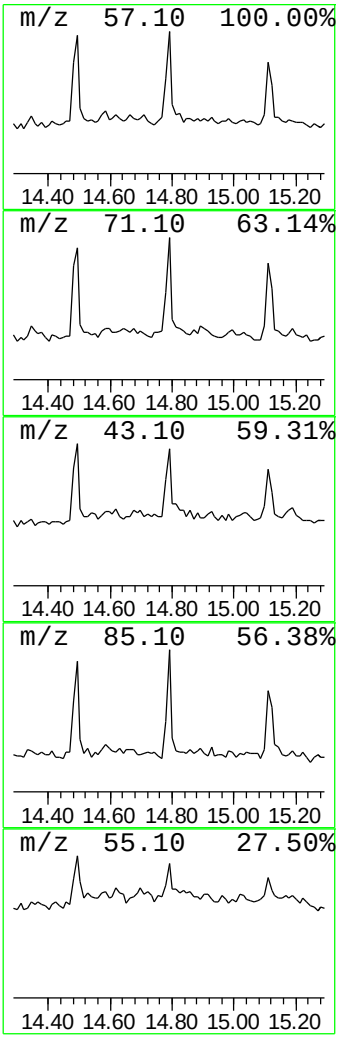
****

Peak Number 8 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.27 ng	60684	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetradecane	198	C14H30	000629-59-4	64
3	Heneicosane	296	C21H44	000629-94-7	53
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	53
5	Octadecane	254	C18H38	000593-45-3	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

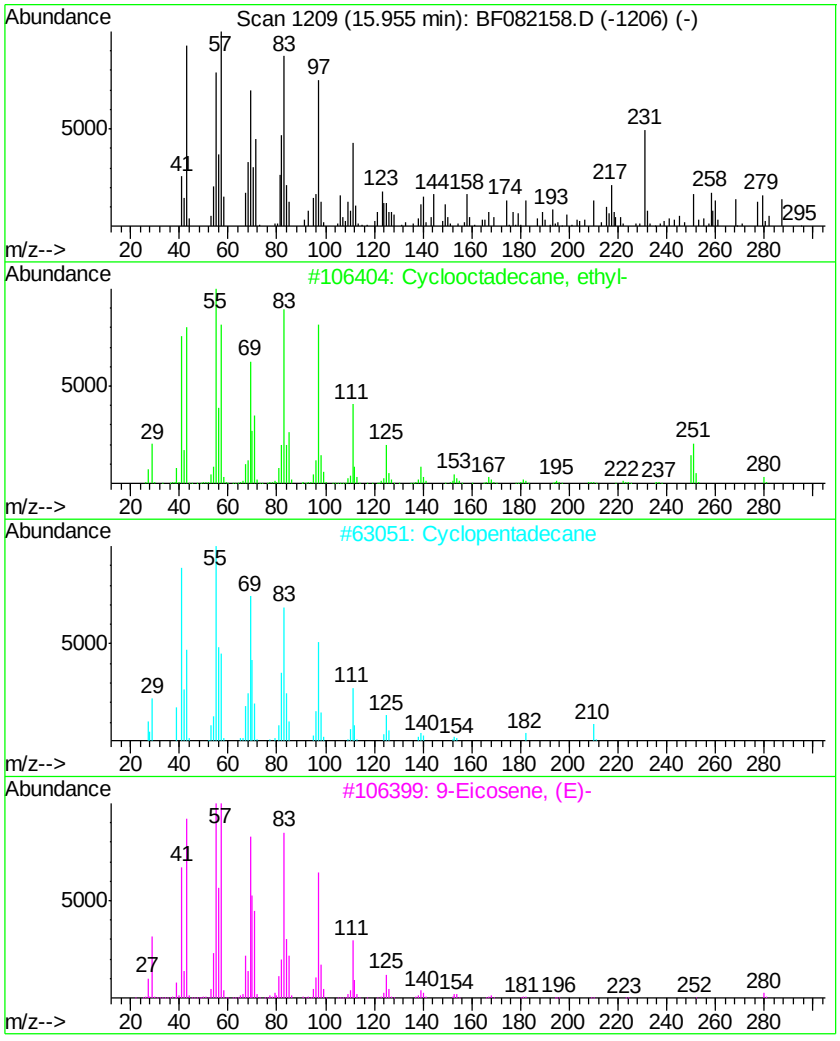
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

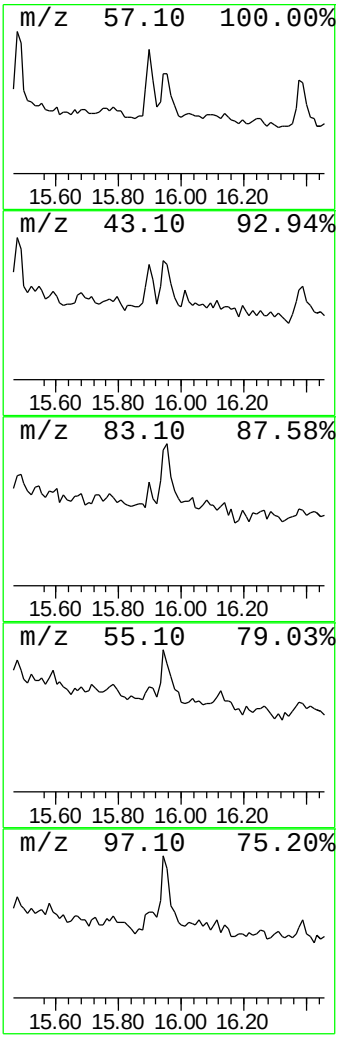
****

Peak Number 10 Cyclooctadecane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.09 ng	82498	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	83
2	Cyclopentadecane	210	C15H30	000295-48-7	58
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	56
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	53
5	1-Hexacosanol	382	C26H54O	000506-52-5	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100915\
Data File : BF082158.D
Acq On : 9 Oct 2015 21:45
Operator : UM/IZ
Sample : G3921-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-COMP(1-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.04	33.3	ng	1003140	1	6.85	603350	20.0
unknown6.62	6.62	65.4	ng	1973310	1	6.85	603350	20.0
Octadecane	10.80	2.8	ng	124900	4	11.38	897380	20.0
n-Hexadecanoic acid	11.91	4.9	ng	220434	4	11.38	897380	20.0
Benzaldehyde, 3,5...	11.99	2.3	ng	105201	4	11.38	897380	20.0
Trichloroacetic a...	13.86	4.1	ng	345940	5	14.02	1687280	20.0
Heptadecane	14.79	2.3	ng	60684	6	15.46	534279	20.0
Cyclooctadecane, ...	15.96	3.1	ng	82498	6	15.46	534279	20.0