LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF060716.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	1.690	7	9	33	rVB	330037	613933	27.98%	2.919%
2	2.684	94	96	113	rBV4	8901	49289	2.25%	0.234%
3	4.673	267	270	286	rBV	218904	469019	21.38%	2.230%
4	5.130	308	310	325	rBV	1076148	1747972	79.66%	8.310%
5	5.542	343	346	349	rBV	20991	28824	1.31%	0.137%
6	6.216	402	405	412	rBV	1335018	1652668	75.32%	7.856%
7	6.319	412	414	432	rVB	1770721	1875339	85.47%	8.915%
8	6.547	432	434	445	rBV	327299	359241	16.37%	1.708%
9	6.696	445	447	450	rBV	1104943	1412765	64.39%	6.716%
10	7.119	482	484	487	rBV	742239	1070558	48.79%	5.089%
11	7.828	544	546	559	rBV	344743	514397	23.44%	2.445%
12	8.913	638	641	643	rBV	2115997	2194212	100.00%	10.431%
13	9.233	666	669	671	rBV2	42064	44165	2.01%	0.210%
14	9.313	674	676	678	rBV	808440	694128	31.63%	3.300%
15	9.576	697	699	701	rBV	666338	608831	27.75%	2.894%
16	9.611	701	702	704	rVB	36908	28156	1.28%	0.134%
17	10.125	743	747	750	rVB2	19437	23739	1.08%	0.113%
18	10.365	765	768	771	rBV	1238077	1399315	63.77%	6.652%
19	10.491	777	779	784	rVB	37938	48889	2.23%	0.232%
20	10.936	816	818	819	rBV	40530	30723	1.40%	0.146%
21	11.051	826	828	833	rBV2	609296	755892	34.45%	3.593%
22	11.131	833	835	838	rVB	38639	48433	2.21%	0.230%
23	11.302	848	850	853	rBV2	17223	23631	1.08%	0.112%
24	11.359	853	855	857	rBV	44122	36357	1.66%	0.173%
25	11.599	873	876	877	rBV2	14429	27510	1.25%	0.131%
26	11.657	880	881	888	rVB2	29250	52620	2.40%	0.250%
27	11.759	888	890	894	rVB2	17318	24370	1.11%	0.116%
28	12.251	931	933	936	rBV	153692	225907	10.30%	1.074%
29	12.479	950	953	956	rBV	199789	236779	10.79%	1.126%
30	12.639	964	967	969	rBV	1631723	2020739	92.09%	9.606%
31	12.697	971	972	976	rVB2	16293	28413	1.29%	0.135%
32	12.811	979	982	985	rBV	21485	37744	1.72%	0.179%
33	12.880	985	988	990	rBV2	36408	45207	2.06%	0.215%
34	12.914	990	991	995	rVB2	18237	25774	1.17%	0.123%

LSC Area Percent Report

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Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.211	1014	1017	1022	rBV2	9892	25949	1.18%	0.123%
36	13.451	1033	1038	1039	rBV2	16669	31211	1.42%	0.148%
37	13.542	1044	1046	1055	rVV2	125522	219995	10.03%	1.046%
38	13.680	1055	1058	1064	rVV2	425210	699289	31.87%	3.324%
39	13.782	1064	1067	1070	rVB	14272	22290	1.02%	0.106%
40	14.068	1087	1092	1093	rBV	18804	27951	1.27%	0.133%
41	14.171	1096	1101	1106	rBV5	76692	171482	7.82%	0.815%
42	14.571	1135	1136	1139	rVB2	23803	29493	1.34%	0.140%
43	14.674	1142	1145	1149	rVV	95341	178590	8.14%	0.849%
44	14.731	1149	1150	1151	rVV	35054	36493	1.66%	0.173%
45	14.765	1151	1153	1158	rVB	52007	89449	4.08%	0.425%
46	14.925	1165	1167	1170	rBV	50819	60968	2.78%	0.290%
47	14.983	1170	1172	1174	rVV	64932	81689	3.72%	0.388%
48	15.028	1174	1176	1182	rVB	297777	412317	18.79%	1.960%
49	15.211	1187	1192	1198	rBV6	19787	50558	2.30%	0.240%
50	15.394	1206	1208	1211	rBV2	29795	42228	1.92%	0.201%
51	15.451	1211	1213	1215	rBV3	19334	40276	1.84%	0.191%
52	16.263	1276	1284	1288	rBV	39709	93596	4.27%	0.445%
53	16.628	1313	1316	1322	rBV	26379	83283	3.80%	0.396%
54	16.743	1323	1326	1331	rVB	31721	66254	3.02%	0.315%
55	18.114	1440	1446	1447	rBV5	9410	27931	1.27%	0.133%
56	18.286	1458	1461	1466	rVB3	15514	43005	1.96%	0.204%
57	19.497	1557	1567	1570	rBV6	8707	45990	2.10%	0.219%

Sum of corrected areas: 21035826

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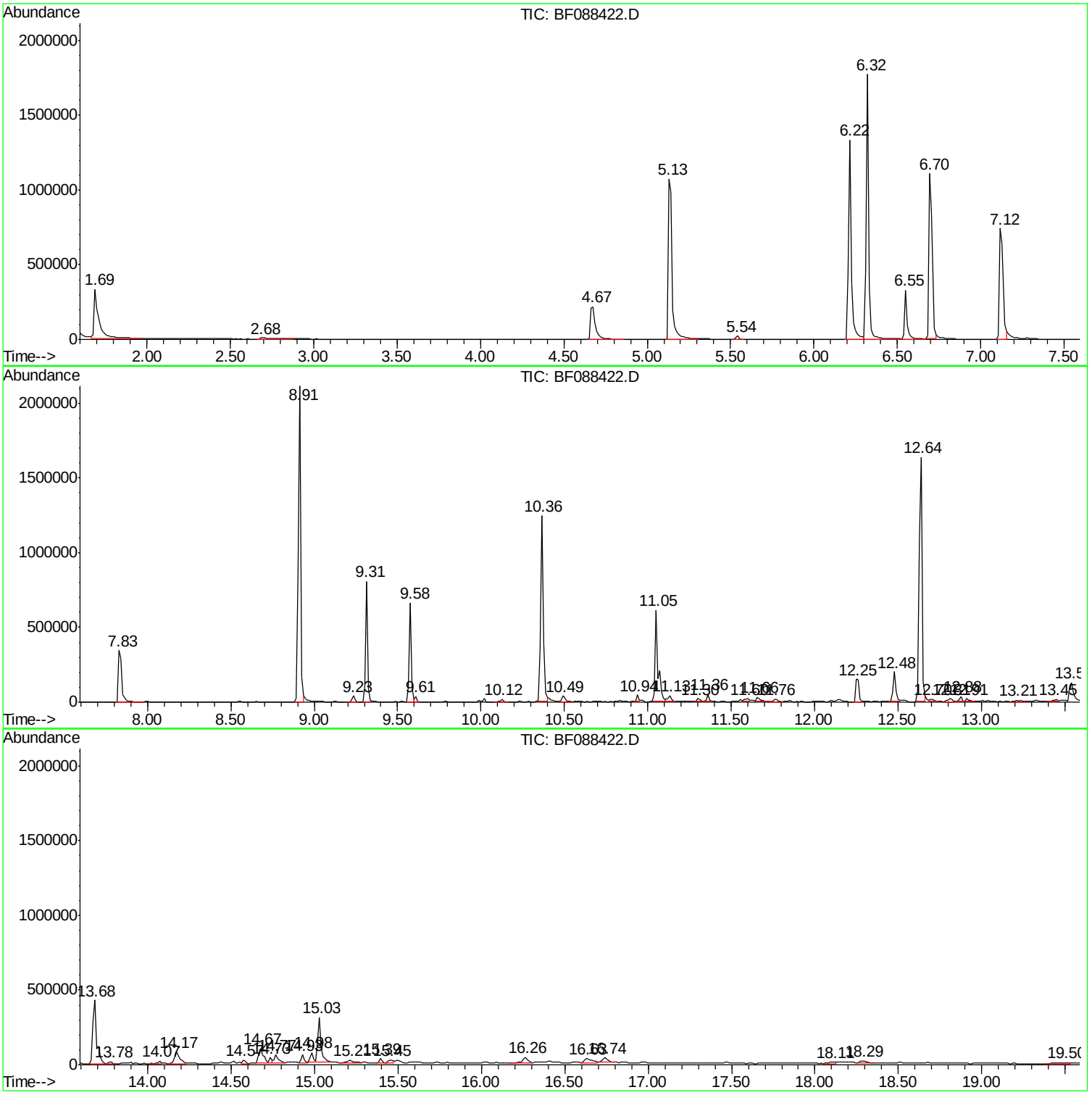
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF088422.D
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Operator : UM/SJ
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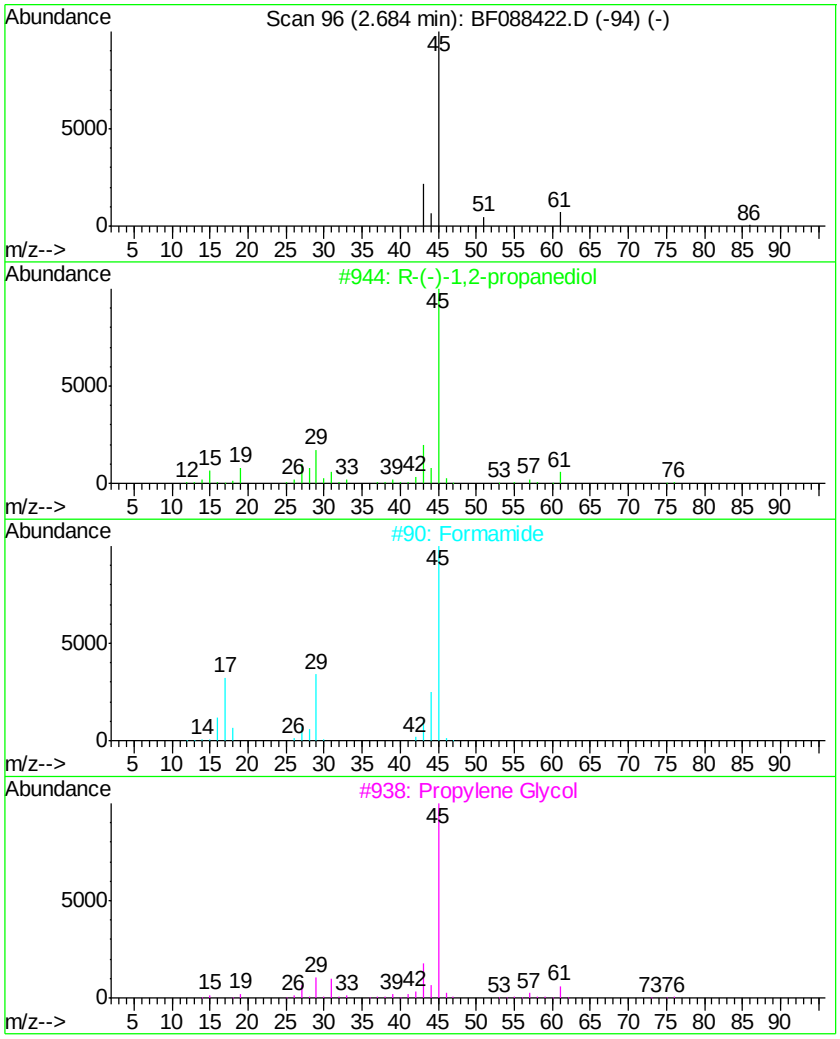
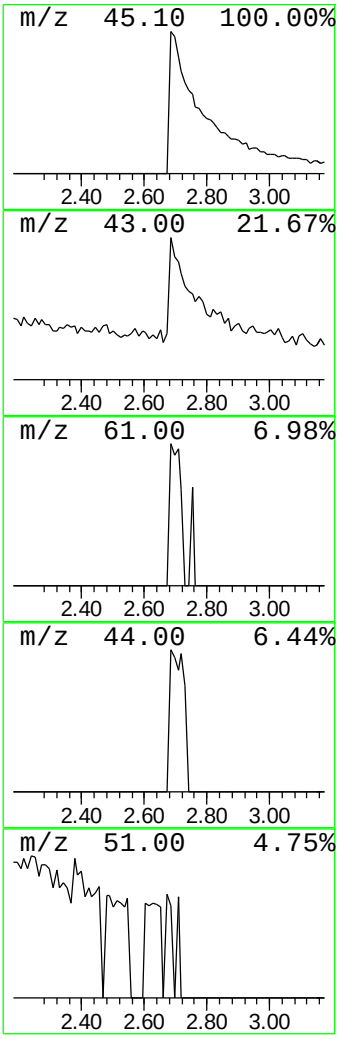
Peak Number 2 unknown2.68 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.68	2.74 ng	49289	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	4
2	Formamide	45	CH3NO	000075-12-7	2
3	Propylene Glycol	76	C3H8O2	000057-55-6	2
4	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	2
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	2





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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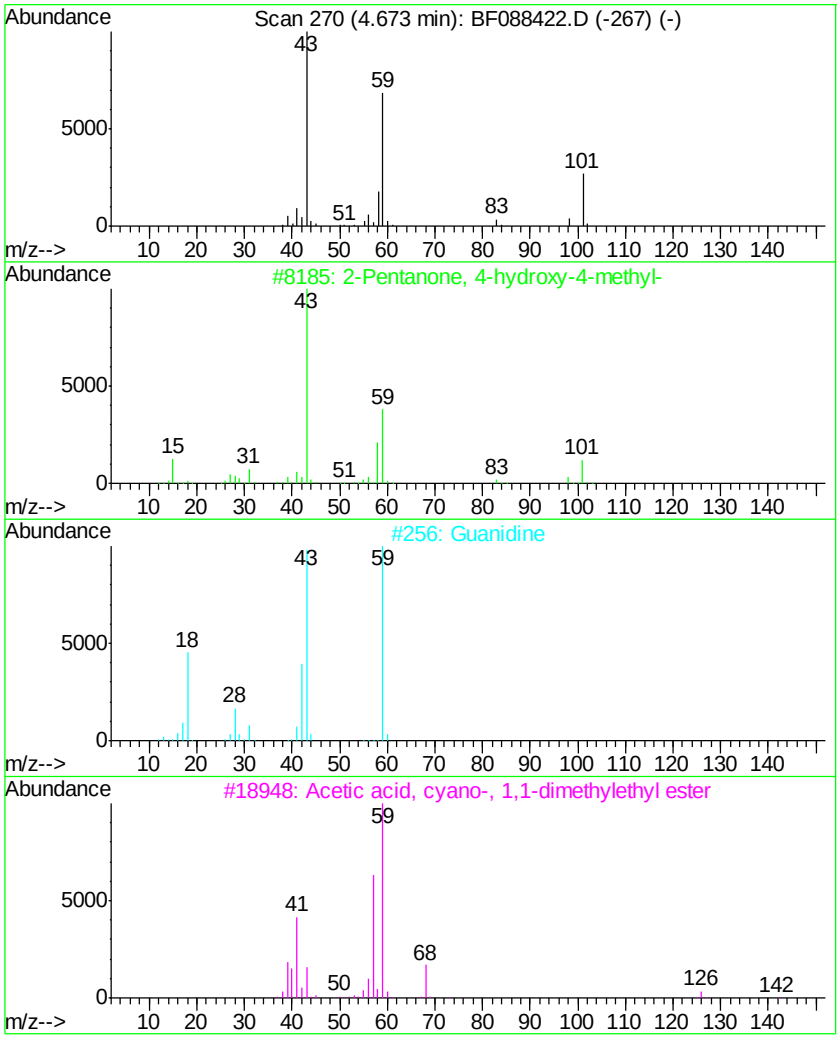
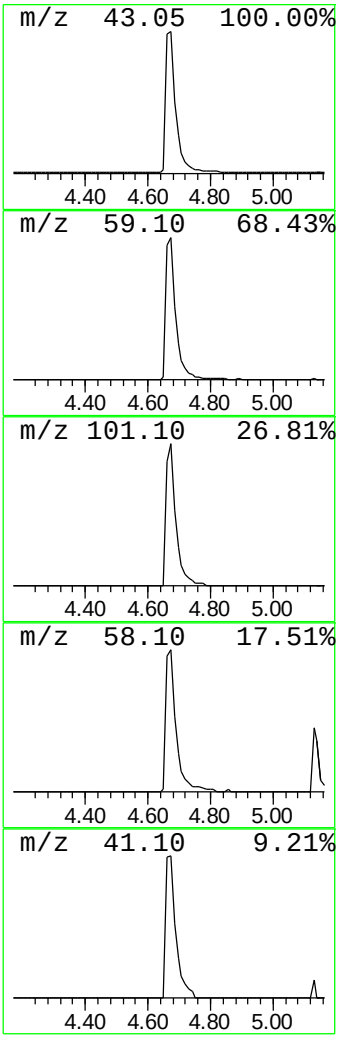
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	26.11 ng	469019	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

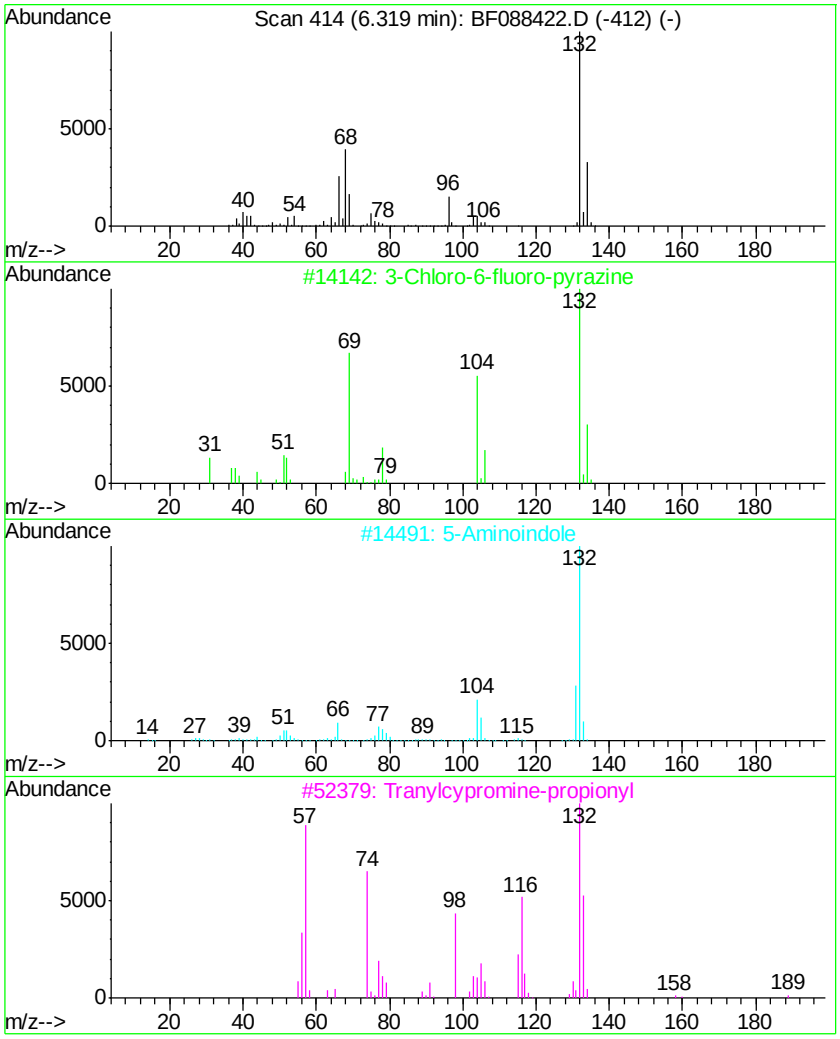
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

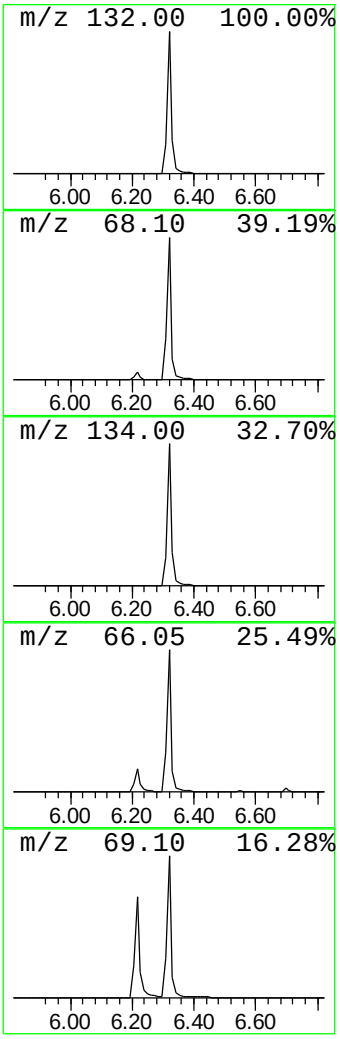
****

Peak Number 4 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	104.41 ng	1875340	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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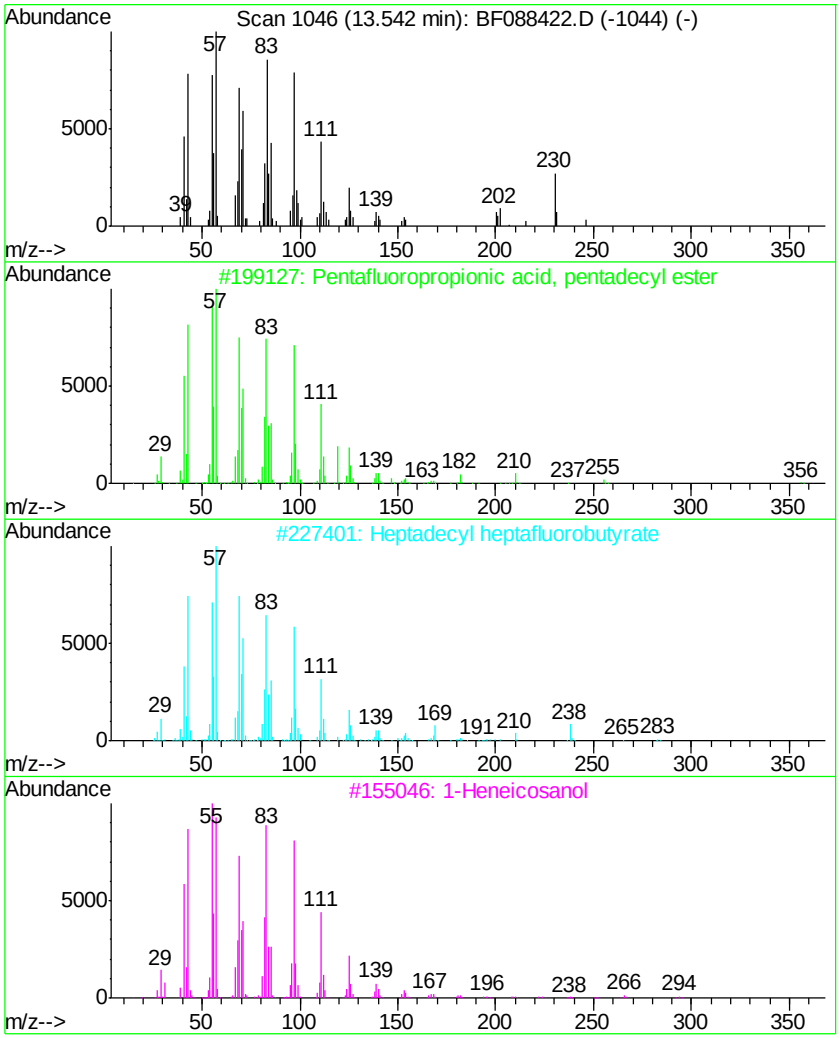
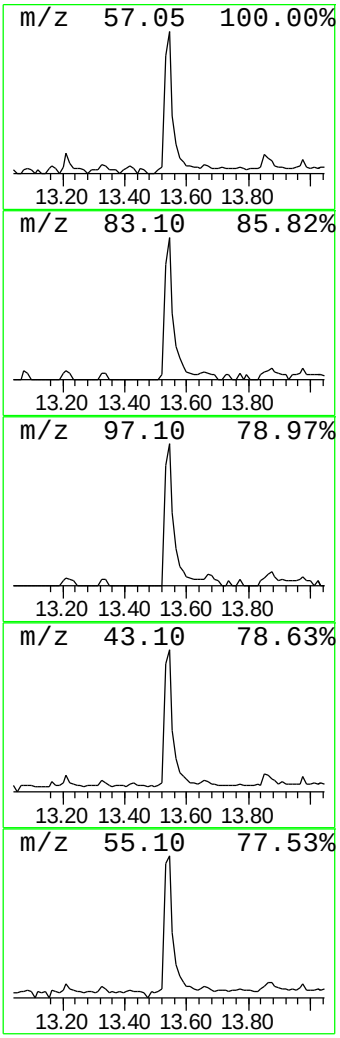
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	6.29 ng	219995	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
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Sample : H3663-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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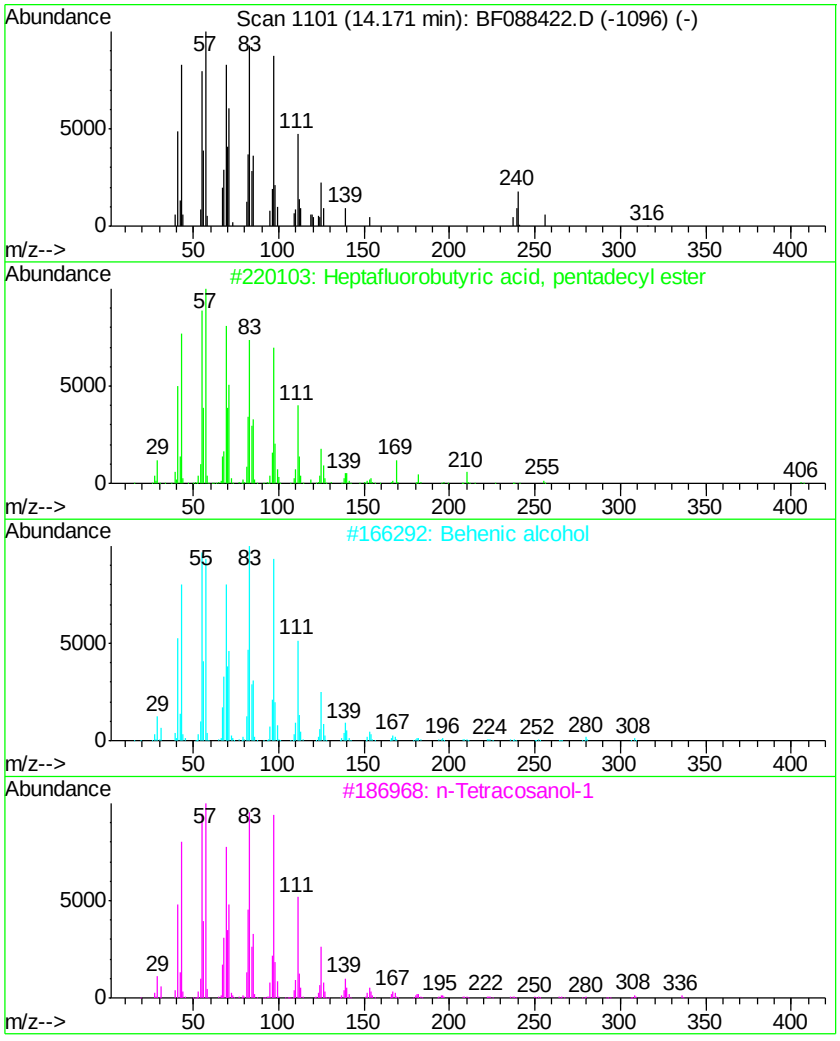
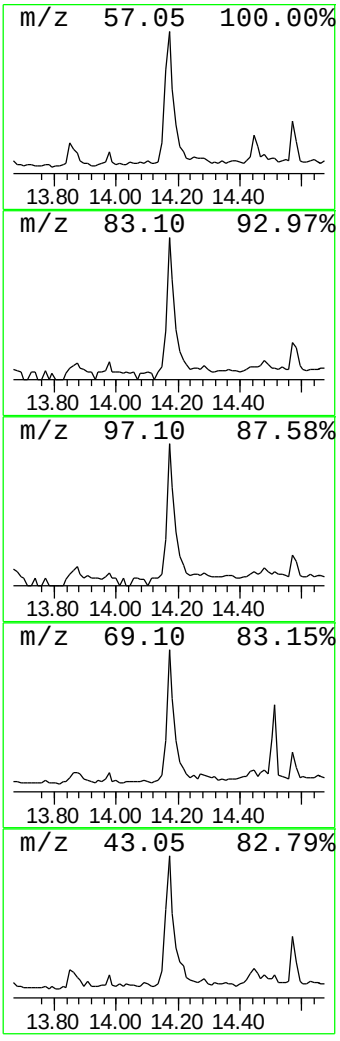
Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	4.90 ng	171482	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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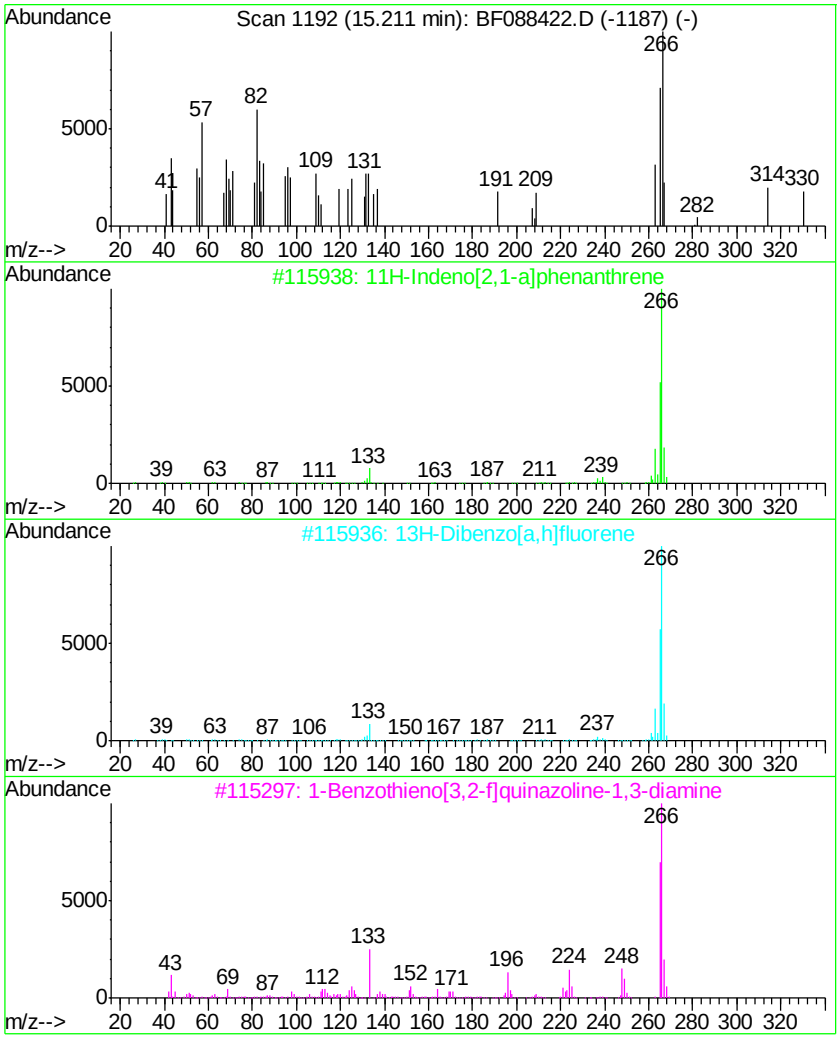
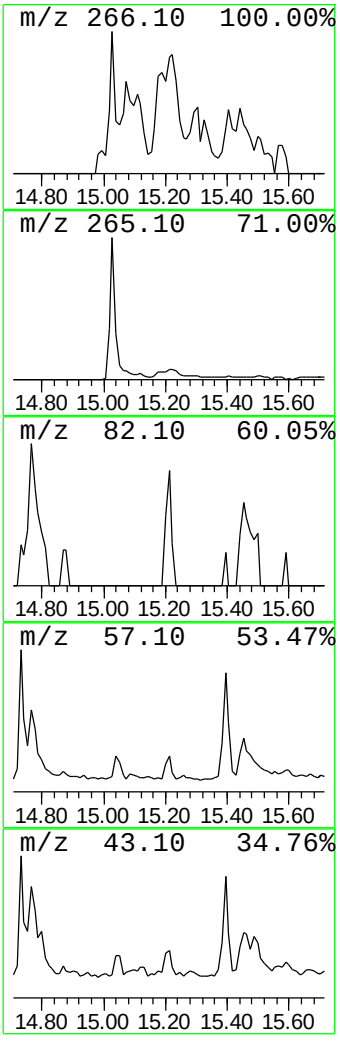
Peak Number 10 unknown15.21 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.45 ng	50558	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Indeno[2,1-a]phenanthrene	266	C21H14	000220-97-3	43
2	13H-Dibenzo[a,h]fluorene	266	C21H14	000239-85-0	43
3	1-Benzothieno[3,2-f]quinazoline-...	266	C14H10N4S	065642-92-4	43
4	Acetic acid, 2-(2-benzyl-1-benzo...	266	C16H14N2O2	152342-26-2	38
5	8H-Indeno[2,1-b]phenanthrene	266	C21H14	000241-28-1	37





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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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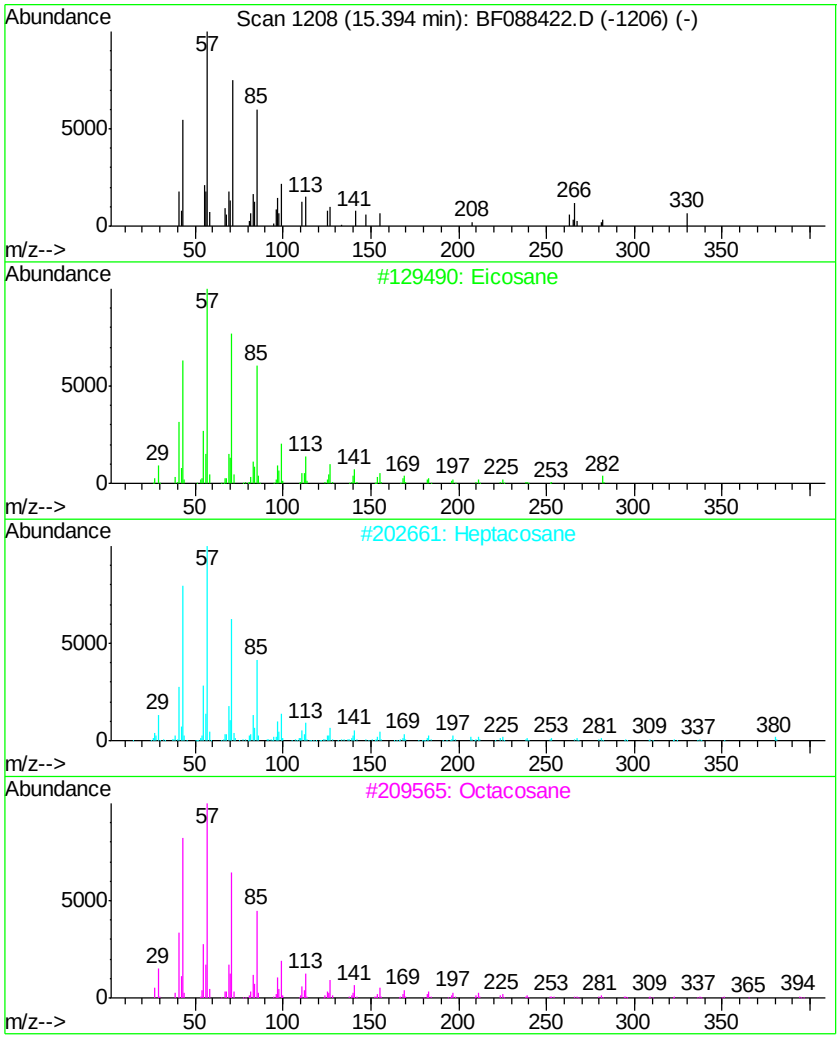
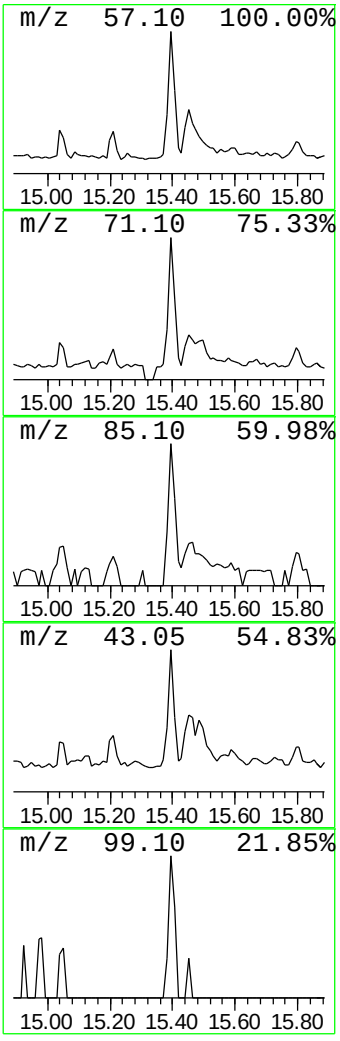
Peak Number 11 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	2.05 ng	42228	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hexatriacontane	507	C36H74	000630-06-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
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Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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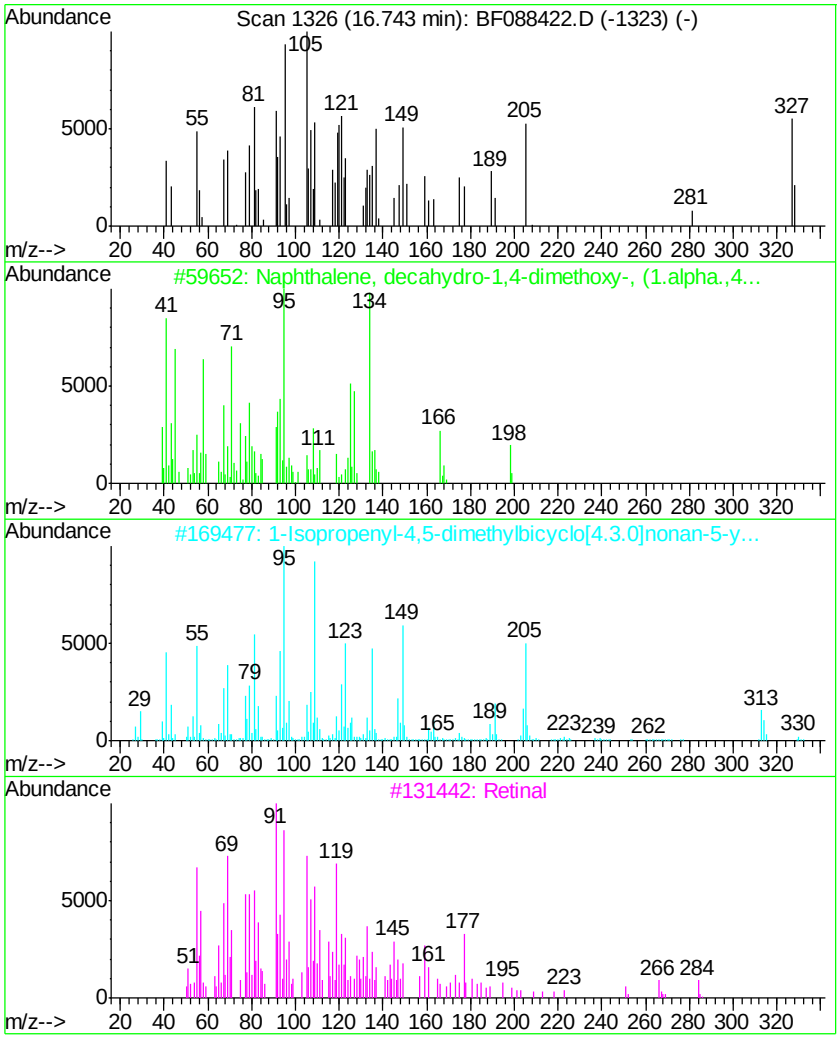
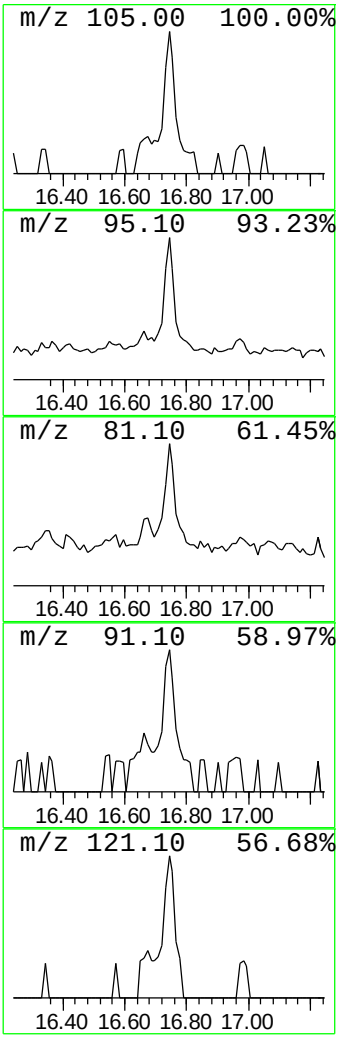
Peak Number 12 Naphthalene, decahydro-1,4-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	3.21 ng	66254	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,4-dimet...	198	C12H22O2	042067-56-1	59
2	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	22
3	Retinal	284	C20H28O	000116-31-4	22
4	1,4-Methanonaphthalene, 6,7-diet...	206	C15H26	016539-02-9	16
5	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

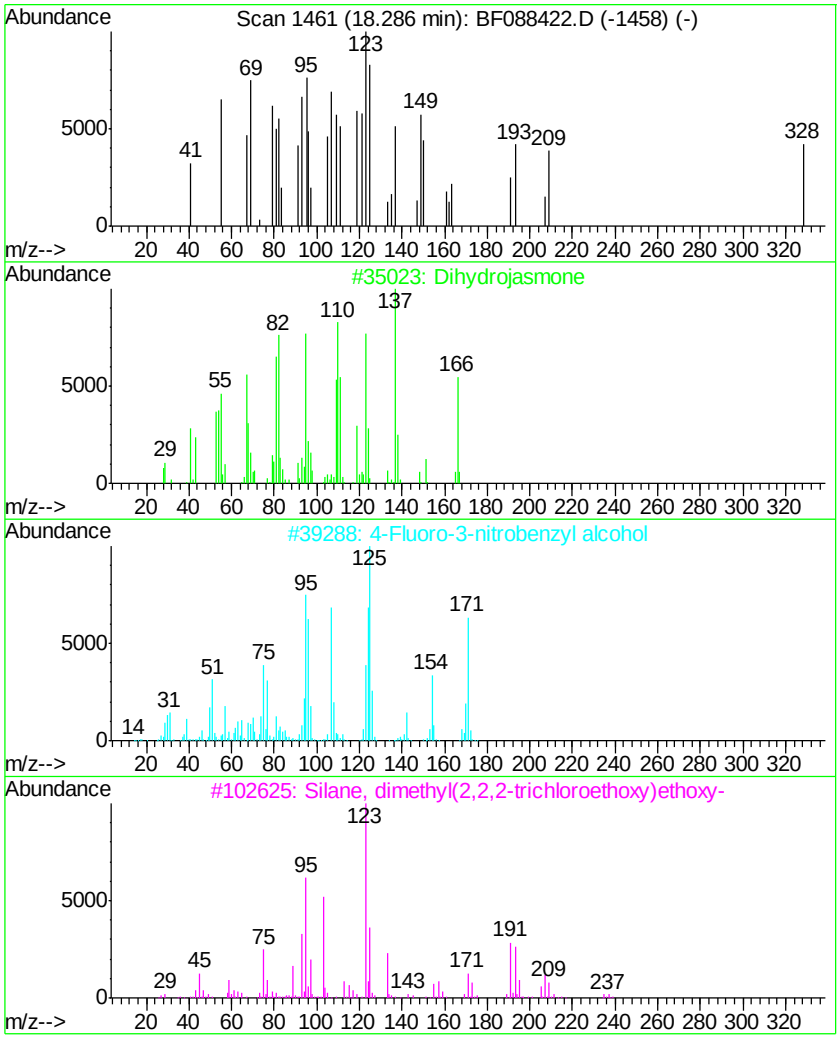
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

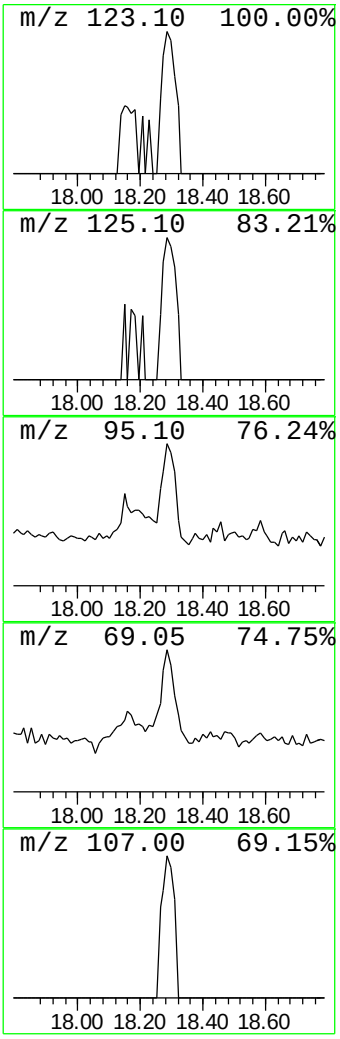
****

Peak Number 13 unknown18.29 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	2.09 ng	43005	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dihydrojasmone	166	C11H18O	001128-08-1	22
2	4-Fluoro-3-nitrobenzyl alcohol	171	C7H6FNO3	020274-69-5	22
3	Silane, dimethyl(2,2,2-trichloro...	250	C6H13Cl3O2Si	1000347-56-1	16
4	4a-Hydroxy-4-nitroperhydronaphth...	213	C10H15NO4	1000195-29-3	14
5	Silane, bromomethyltripropyl-	250	C10H23BrSi	1000149-29-6	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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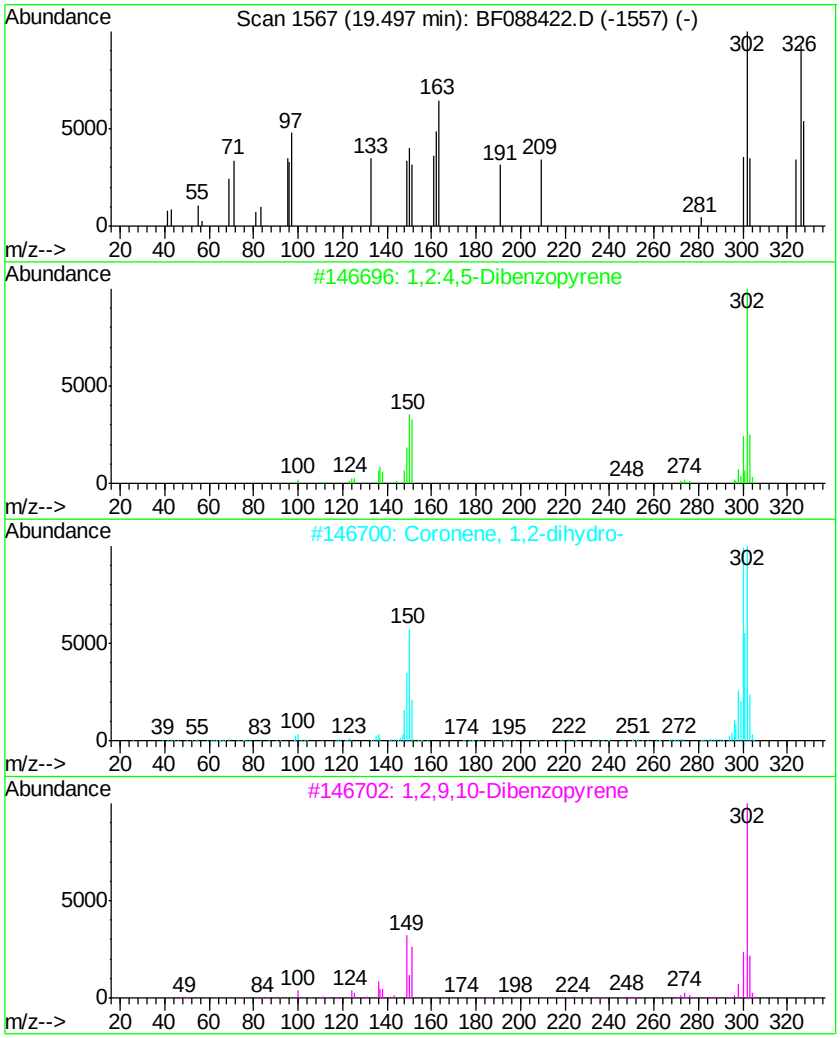
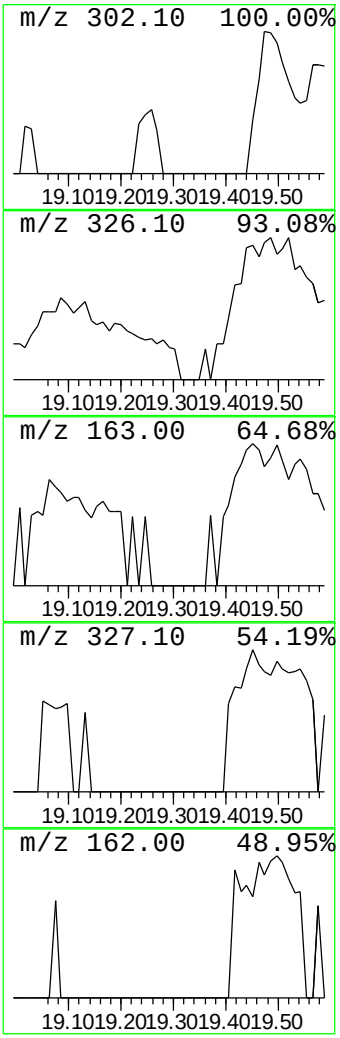
Peak Number 14 unknown19.50 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.50	2.23 ng	45990	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	14
2	Coronene, 1,2-dihydro-	302	C24H14	107716-56-3	10
3	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	9
4	1,1-Dimethyl-4a-hydroxymethyldec...	212	C13H24O2	1000196-01-9	9
5	6-Hydroxy-7-isopropyl-1,4a-dimet...	302	C20H30O2	022595-48-8	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062616\
Data File : BF088422.D
Acq On : 26 Jun 2016 17:01
Operator : UM/SJ
Sample : H3663-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.68	2.68	2.7	ng	49289	1	6.55	359241	20.0
2-Pentanone, 4-hy...	4.67	26.1	ng	469019	1	6.55	359241	20.0
unknown6.32	6.32	104.4	ng	1875340	1	6.55	359241	20.0
Pentafluoropropio...	13.54	6.3	ng	219995	5	13.68	699289	20.0
Heptafluorobutyri...	14.17	4.9	ng	171482	5	13.68	699289	20.0
unknown15.21	15.21	2.5	ng	50558	6	15.03	412317	20.0
Eicosane	15.39	2.0	ng	42228	6	15.03	412317	20.0
Naphthalene, deca...	16.74	3.2	ng	66254	6	15.03	412317	20.0
unknown18.29	18.29	2.1	ng	43005	6	15.03	412317	20.0
unknown19.50	19.50	2.2	ng	45990	6	15.03	412317	20.0