LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF070916\
Data File : BF088867.D
Acq On : 9 Jul 2016 13:15
Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

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-BF063016.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	1.678	7	8	17	rVV	83694	186125	7.48%	0.875%
2	1.804	17	19	26	rVB	784905	925851	37.20%	4.354%
3	4.856	283	286	289	rBV	112517	135445	5.44%	0.637%
4	5.302	322	325	328	rBV	861421	785768	31.57%	3.696%
5	6.353	414	417	419	rBV	710466	620723	24.94%	2.919%
6	6.479	426	428	431	rVB	1089226	1362585	54.75%	6.408%
7	6.719	446	449	451	rBV	605160	505880	20.33%	2.379%
8	6.879	460	463	465	rVB	1372304	1466207	58.91%	6.896%
9	7.279	496	498	500	rBV	892954	1146721	46.08%	5.393%
10	7.999	559	561	563	rBV	617979	643302	25.85%	3.025%
11	8.365	591	593	598	rBV3	24793	46546	1.87%	0.219%
12	8.936	640	643	650	rVB3	10426	30234	1.21%	0.142%
13	9.085	653	656	658	rBV	2547094	2488729	100.00%	11.705%
14	9.119	658	659	662	rVB	41757	34955	1.40%	0.164%
15	9.473	688	690	692	rBV	65795	52612	2.11%	0.247%
16	9.748	712	714	717	rVB2	680928	872826	35.07%	4.105%
17	9.976	728	734	737	rBV2	25299	43978	1.77%	0.207%
18	10.091	742	744	746	rBV	40608	35667	1.43%	0.168%
19	10.536	780	783	786	rBV	1363359	1332549	53.54%	6.267%
20	10.674	791	795	798	rBV	25488	51428	2.07%	0.242%
21	10.731	798	800	801	rVV	28517	28843	1.16%	0.136%
22	10.765	801	803	804	rVV	38930	45653	1.83%	0.215%
23	10.788	804	805	807	rVV2	25422	42213	1.70%	0.199%
24	10.879	809	813	814	rVV2	22446	58796	2.36%	0.277%
25	10.902	814	815	817	rVV2	52182	70792	2.84%	0.333%
26	10.936	817	818	821	rVV2	25788	53640	2.16%	0.252%
27	10.982	821	822	825	rVB	37603	39787	1.60%	0.187%
28	11.119	830	834	835	rBV	48875	71884	2.89%	0.338%
29	11.234	841	844	846	rVB	599021	817391	32.84%	3.844%
30	11.291	846	849	854	rBV2	12583	33594	1.35%	0.158%
31	11.416	857	860	862	rVB3	45384	79746	3.20%	0.375%
32	11.542	869	871	874	rVV	40064	36304	1.46%	0.171%
33	11.645	877	880	882	rVB2	42011	57879	2.33%	0.272%
34	11.782	889	892	894	rBV	459325	574043	23.07%	2.700%

LSC Area Percent Report

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Data File : BF088867.D
Acq On : 9 Jul 2016 13:15
Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.422	945	948	950	rBV	46158	71302	2.86%	0.335%
36	12.479	950	953	956	rVV4	21499	58113	2.34%	0.273%
37	12.571	956	961	963	rVV	694147	1040658	41.81%	4.894%
38	12.651	966	968	971	rVB2	32083	65017	2.61%	0.306%
39	12.811	979	982	985	rBV	1640153	2199672	88.39%	10.345%
40	13.348	1027	1029	1035	rVB3	18648	50933	2.05%	0.240%
41	13.657	1053	1056	1058	rBV	22800	37630	1.51%	0.177%
42	13.725	1058	1062	1065	rVB	170708	285473	11.47%	1.343%
43	13.851	1070	1073	1075	rBV	791465	693052	27.85%	3.259%
44	13.954	1075	1082	1088	rBV6	26843	92905	3.73%	0.437%
45	14.342	1114	1116	1120	rVB	18387	28305	1.14%	0.133%
46	14.640	1140	1142	1144	rBV	38419	42095	1.69%	0.198%
47	14.708	1145	1148	1153	rVB2	44553	76528	3.07%	0.360%
48	15.223	1190	1193	1196	rBV	379610	463560	18.63%	2.180%
49	15.863	1245	1249	1254	rBV	242292	488549	19.63%	2.298%
50	16.034	1260	1264	1267	rBV2	175838	315499	12.68%	1.484%
51	16.080	1267	1268	1275	rVB3	63332	115606	4.65%	0.544%
52	16.263	1281	1284	1287	rBV2	16015	25494	1.02%	0.120%
53	16.571	1307	1311	1314	rVB	49078	91509	3.68%	0.430%
54	16.834	1330	1334	1346	rVB3	39396	124566	5.01%	0.586%
55	17.074	1351	1355	1358	rVB4	22512	55393	2.23%	0.261%
56	17.143	1358	1361	1366	rBV5	10819	36921	1.48%	0.174%
57	17.806	1412	1419	1423	rBV7	7454	25321	1.02%	0.119%

Sum of corrected areas: 21262797

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Misc :
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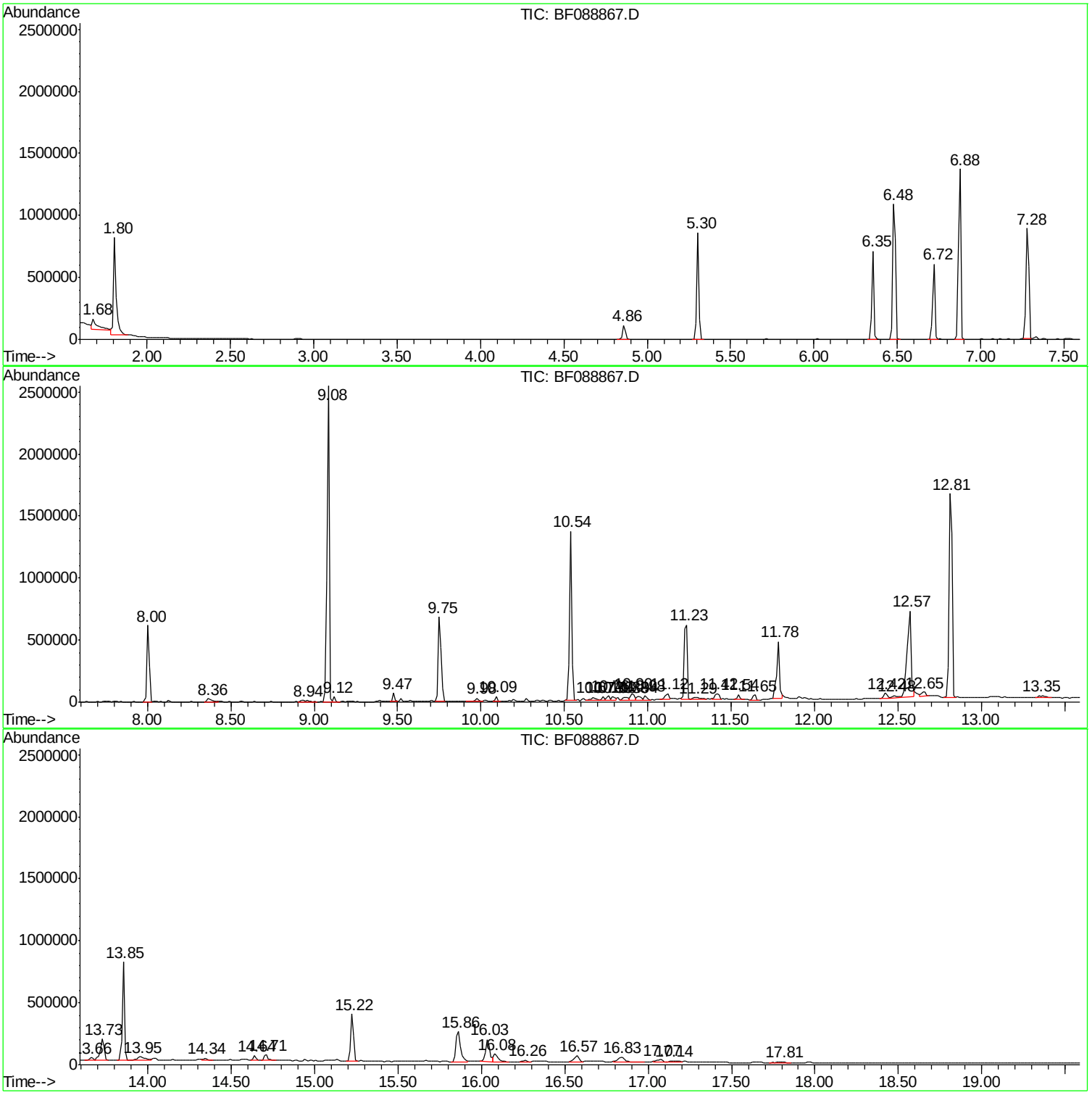
Instrument :
BNA_F
ClientSampleId :
P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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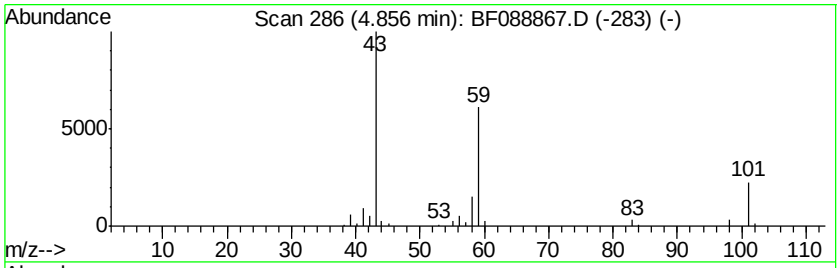
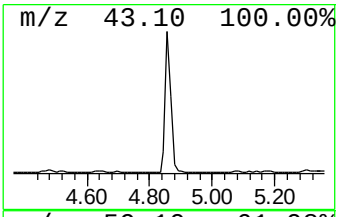
TIC Integration Parameters: LSCINT.P

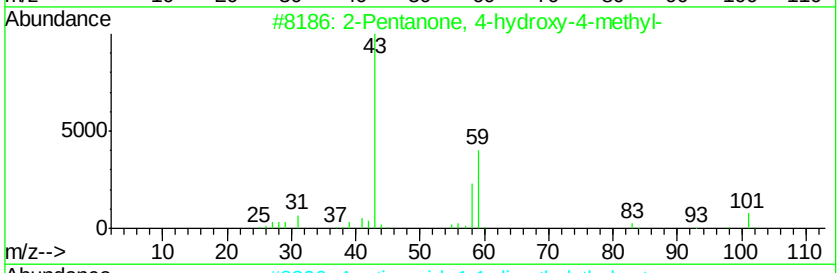
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

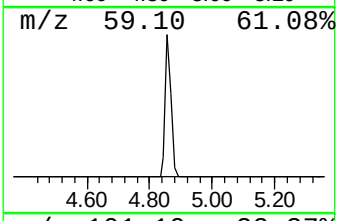
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	5.35 ng	135445	1,4-Dichlorobenzene-d4	6.72

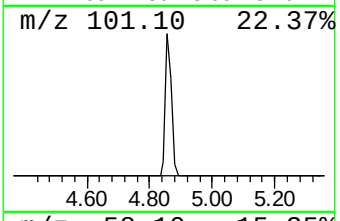
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23

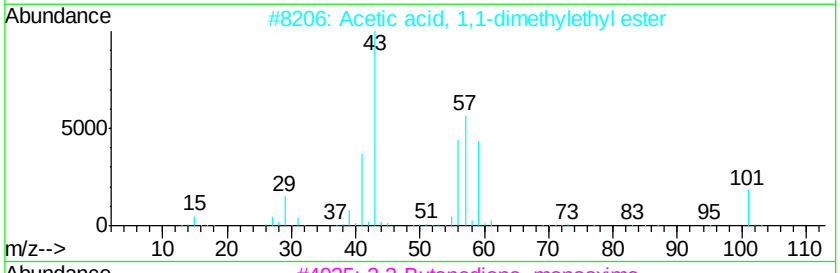


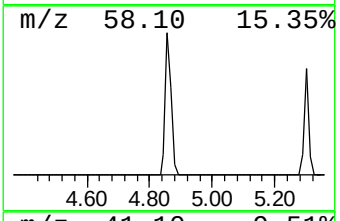


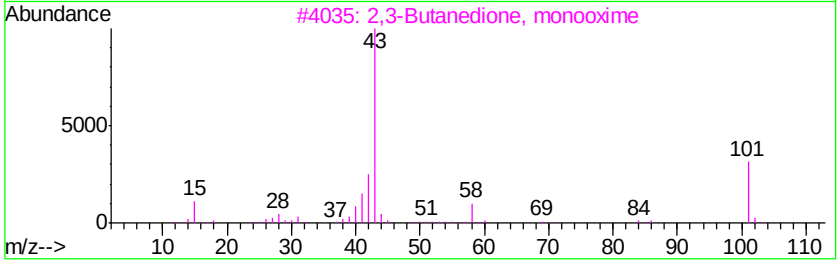


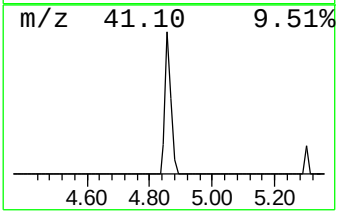












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Acq On : 9 Jul 2016 13:15
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Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

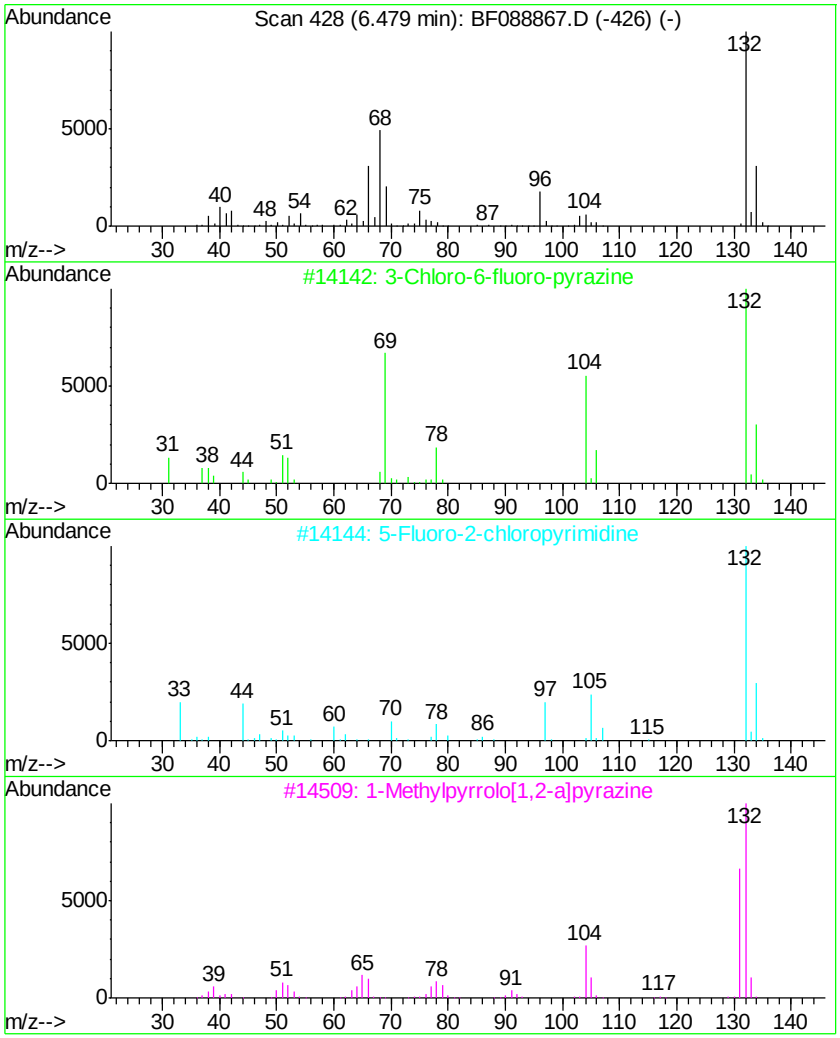
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

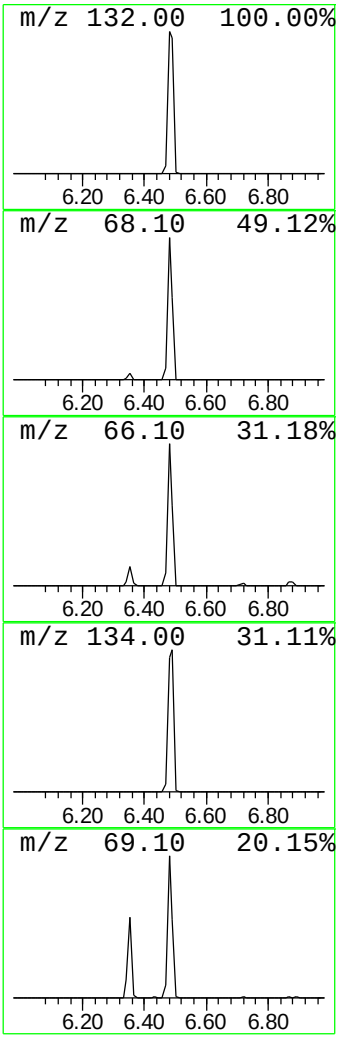
****

Peak Number 4 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	53.87 ng	1362590	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	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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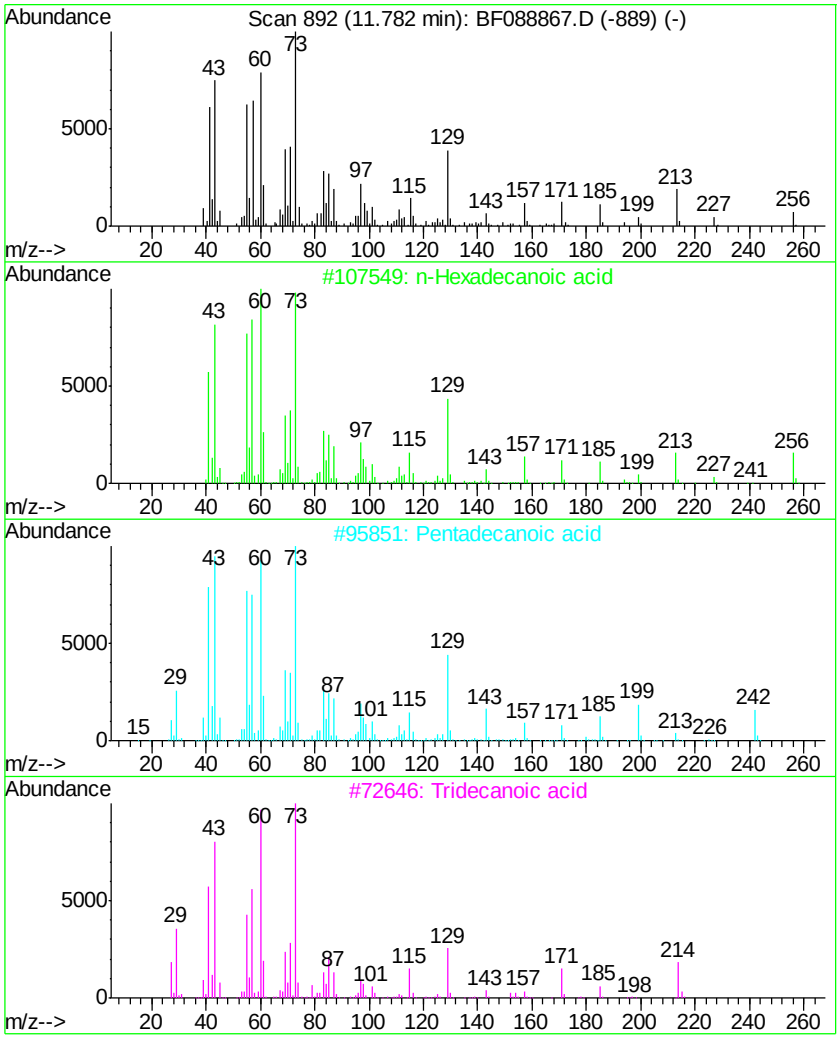
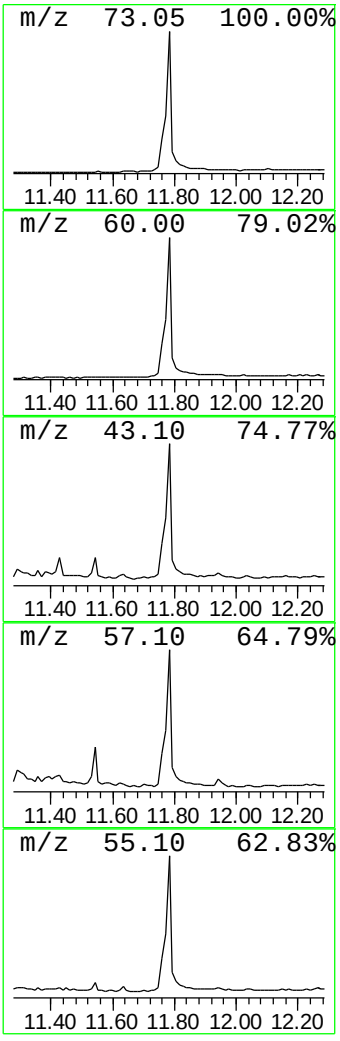
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	14.05 ng	574043	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

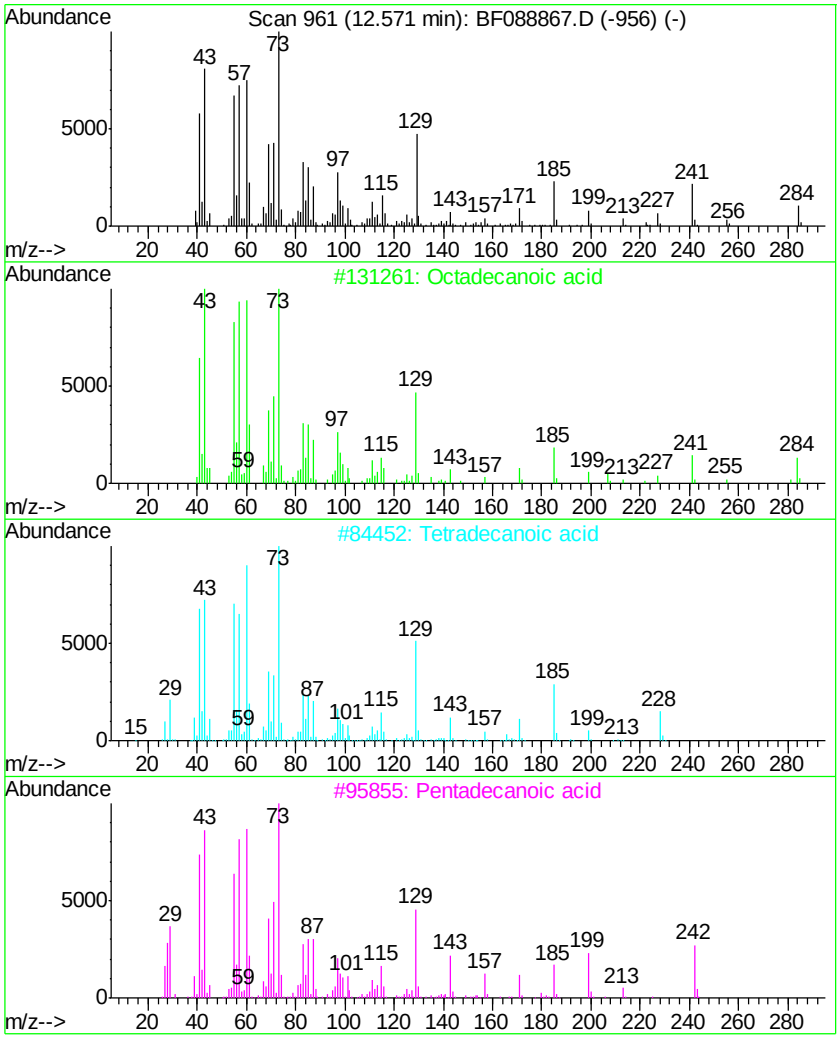
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

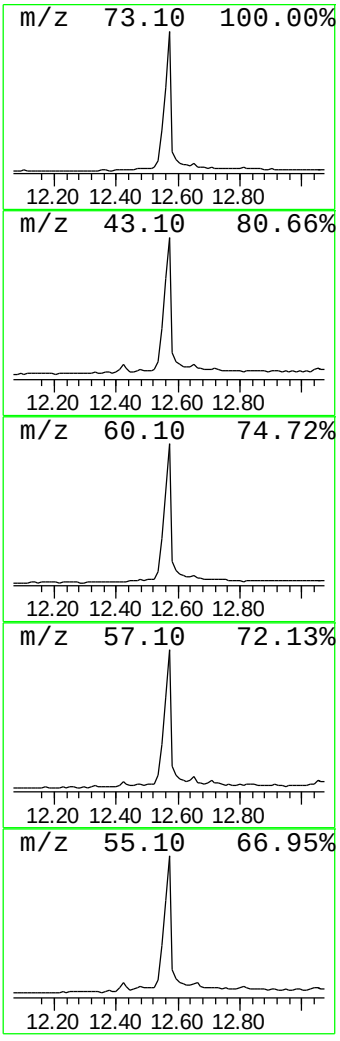
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	30.03 ng	1040660	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Acq On : 9 Jul 2016 13:15
Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

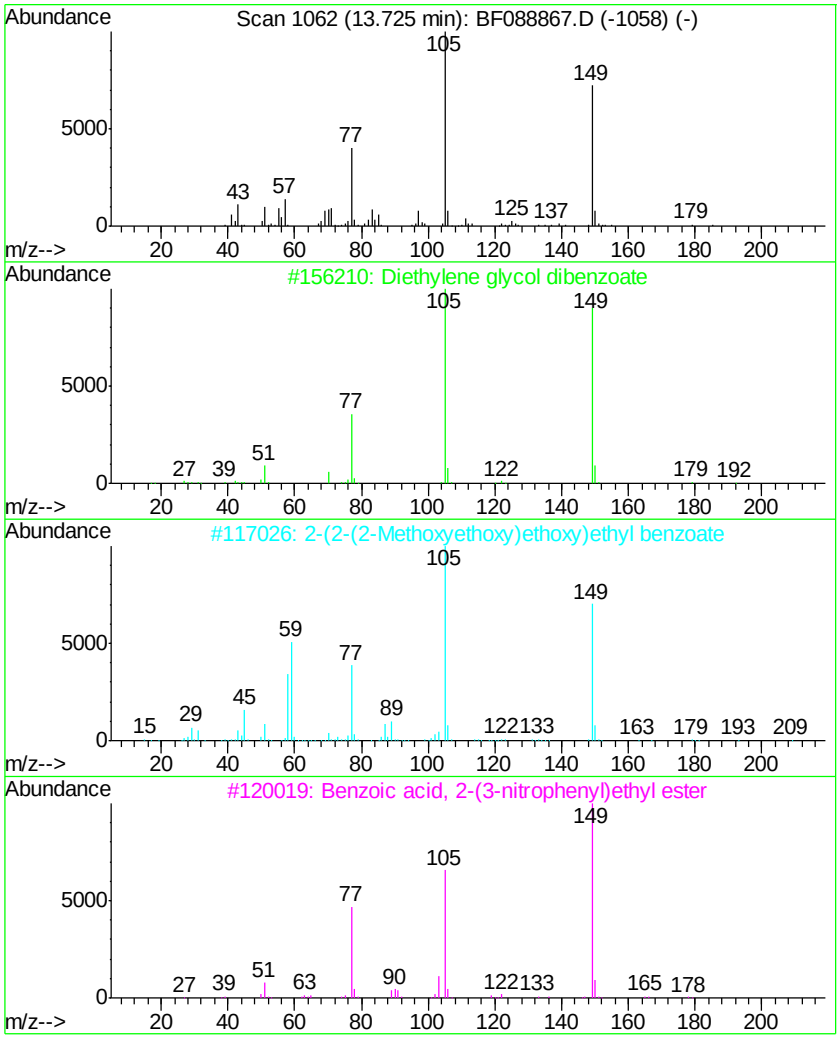
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

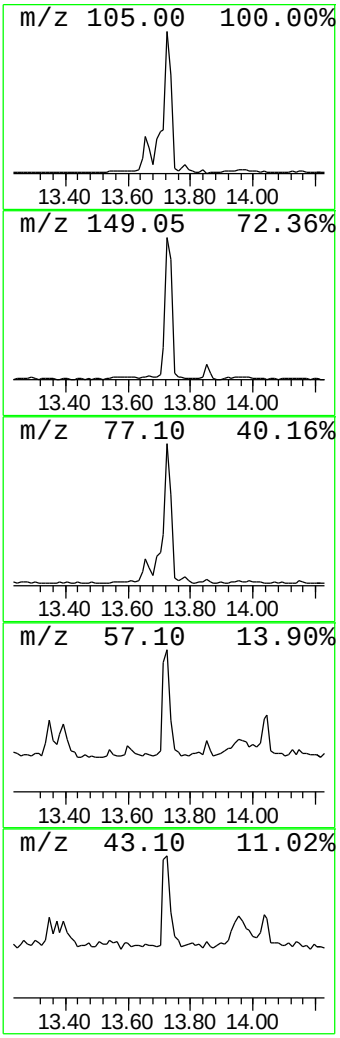
****

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	8.24 ng	285473	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
3	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	59
4	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	50
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	47





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Sample : H3813-26
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

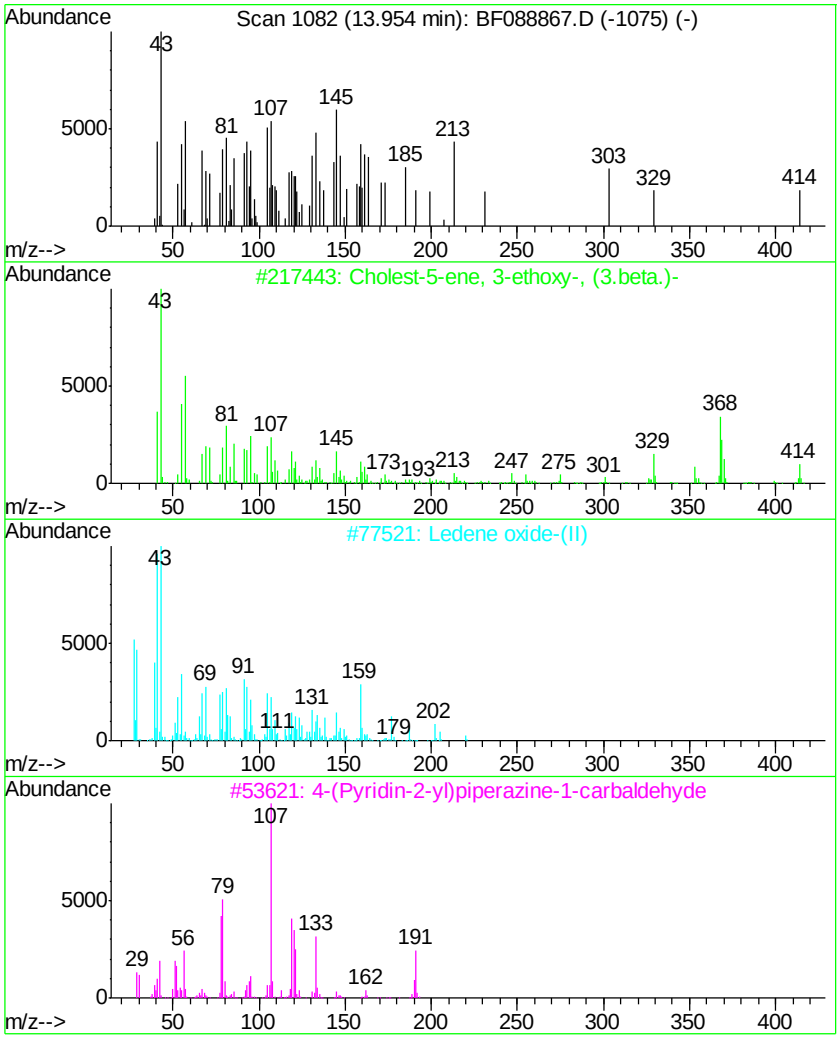
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

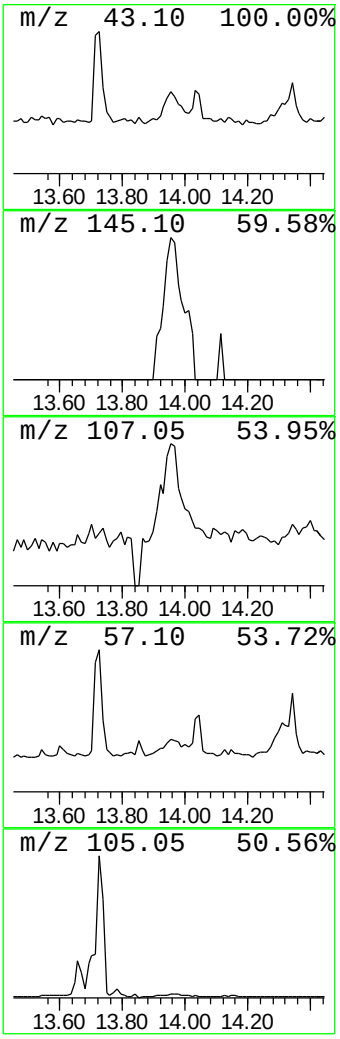
****

Peak Number 9 unknown13.95 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.68 ng	92905	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	38
2	Ledene oxide-(II)	220	C15H24O	1000159-36-7	16
3	4-(Pyridin-2-yl)piperazine-1-car...	191	C10H13N3O	1000368-49-0	10
4	1-Cyclohexene-1-acetaldehyde, 2,...	166	C11H18O	000472-66-2	10
5	Cyclohexane, 1,5-diethenyl-2,3-d...	164	C12H20	068779-14-6	10





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Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

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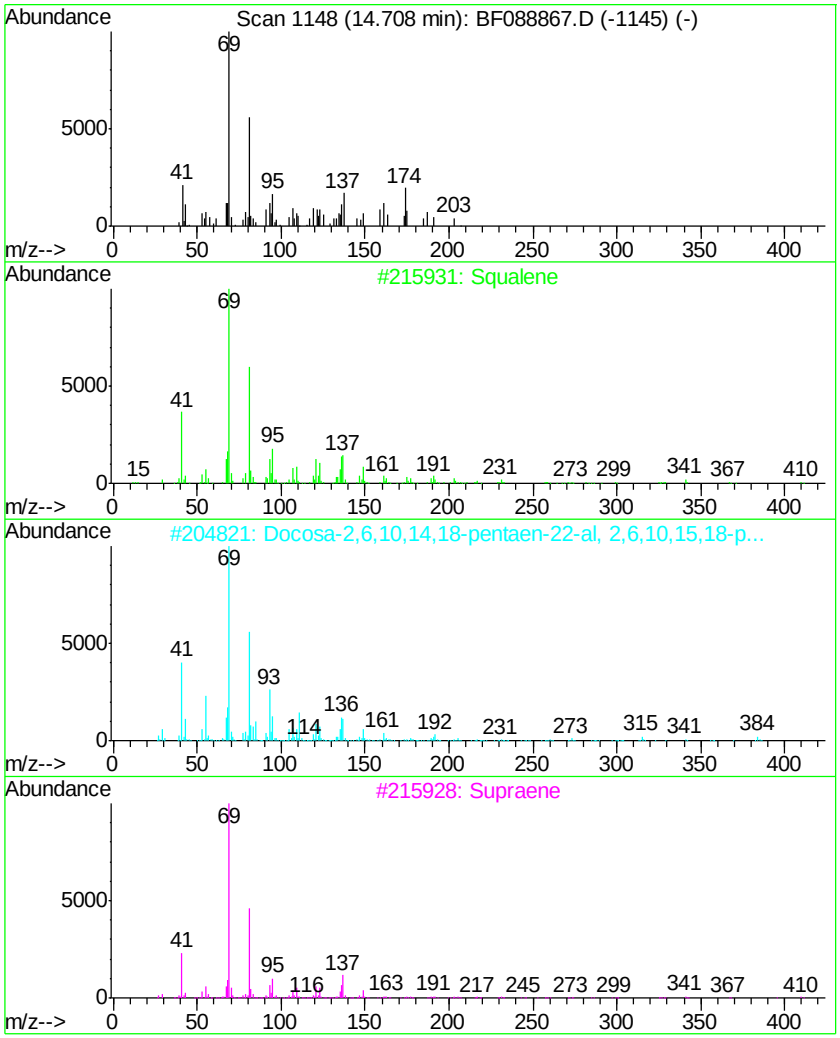
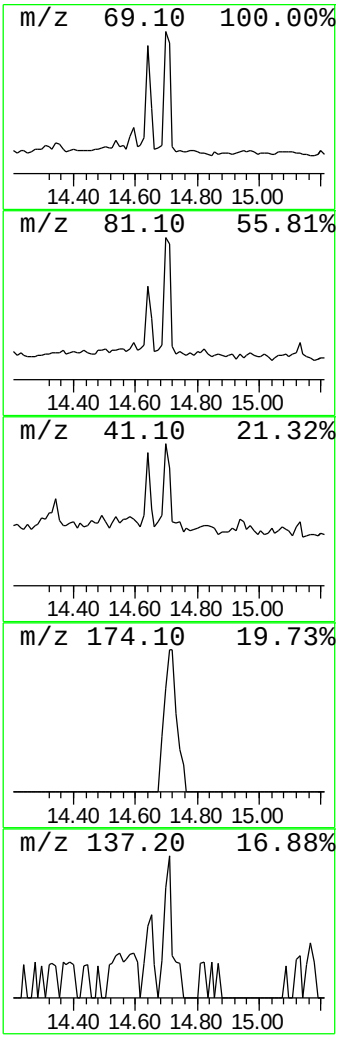
****

Peak Number 10 Squalene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.30 ng	76528	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	68
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	58
3	Supraene	410	C30H50	007683-64-9	58
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	58
5	Farnesol, acetate	264	C17H28O2	1000352-67-2	50





Data Path : V:\HPCHEM1\BNA F\DATA\BF070916\
Data File : BF088867.D
Acq On : 9 Jul 2016 13:15
Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

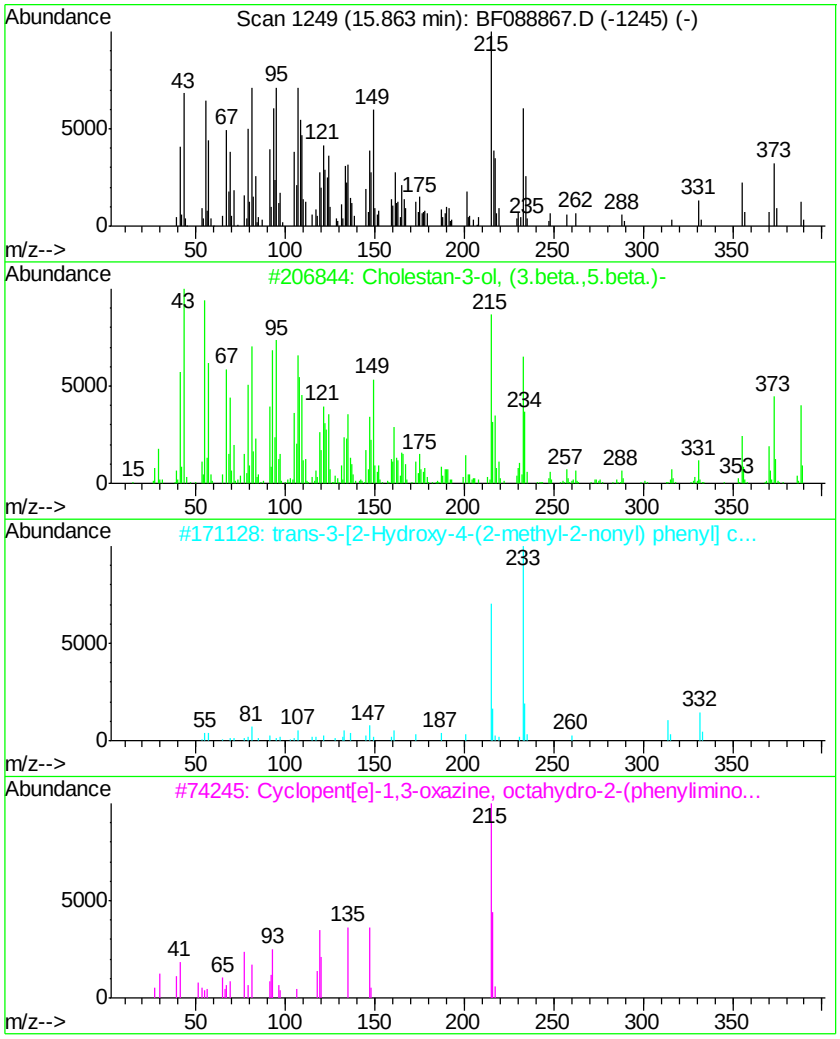
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

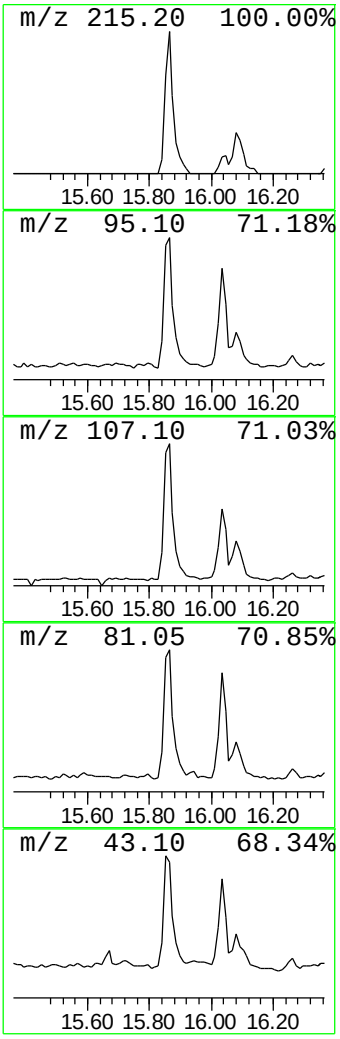
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	21.08 ng	488549	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	89
2	trans-3-[2-Hydroxy-4-(2-methyl-2...	332	C22H36O2	1000370-41-7	38
3	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	30
4	Cholestan-3.alpha.-ol acetate	430	C29H50O2	1000214-83-2	25
5	Cholestanol	388	C27H48O	000080-97-7	25





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Operator : UM/SJ
Sample : H3813-26
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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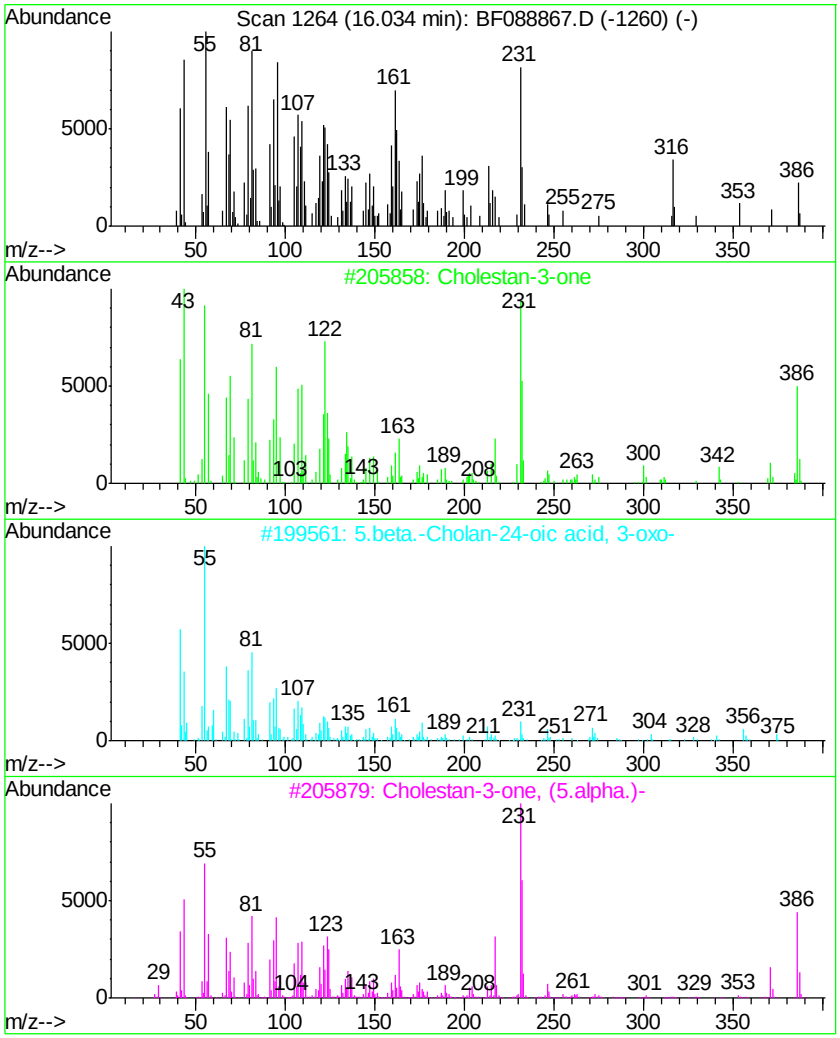
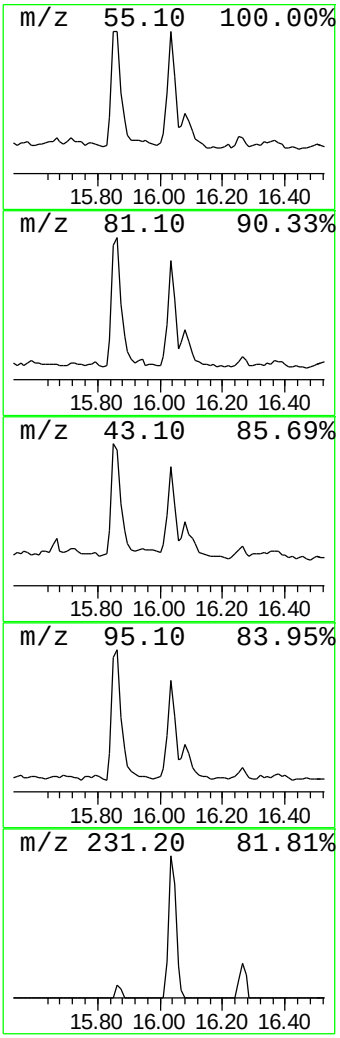
Peak Number 12 Cholestan-3-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	13.61 ng	315499	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-one	386	C27H46O	015600-08-5	64
2	5.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	49
3	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	45
4	Cholestan-2-one	386	C27H46O	1000210-43-4	38
5	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	25





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Acq On : 9 Jul 2016 13:15
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Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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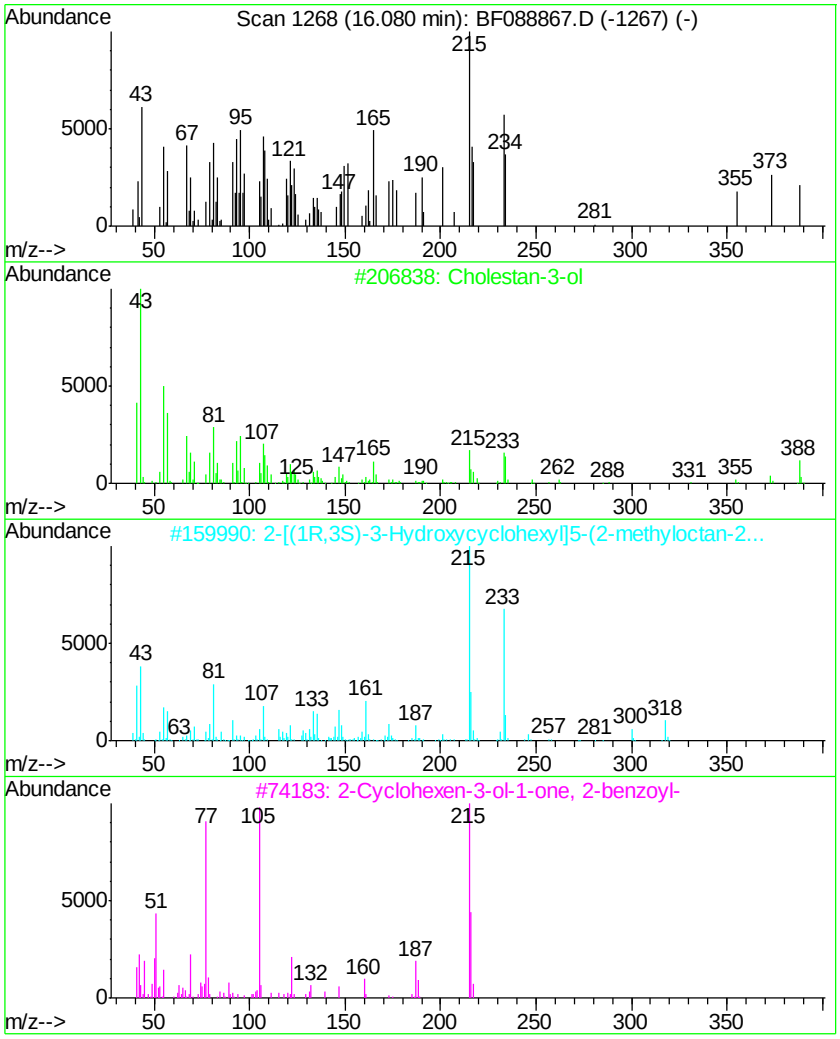
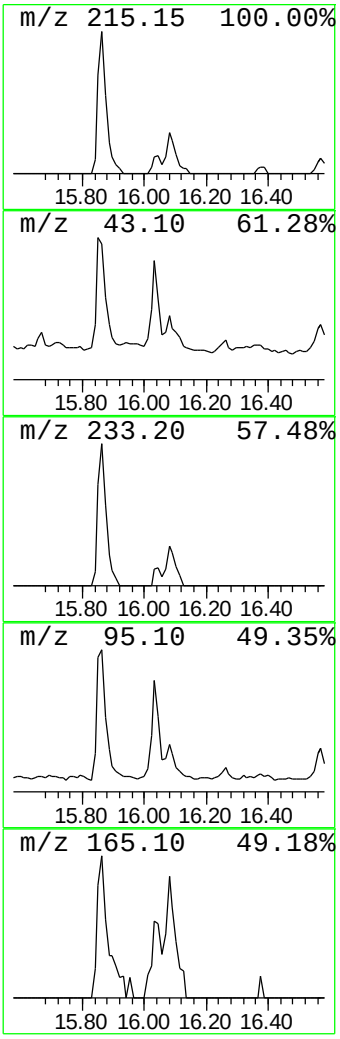
Peak Number 13 Cholestan-3-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	4.99 ng	115606	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol	388	C27H48O	027409-41-2	50
2	2-[(1R,3S)-3-Hydroxycyclohexyl]5...	318	C21H34O2	070434-82-1	16
3	2-Cyclohexen-3-ol-1-one, 2-benzoyl-	216	C13H12O3	061834-43-3	14
4	Kinetin	215	C10H9N5O	000525-79-1	11
5	2,7-Dimethyl-3,5-dimethylthio-2H...	215	C8H13N3S2	066425-11-4	11





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Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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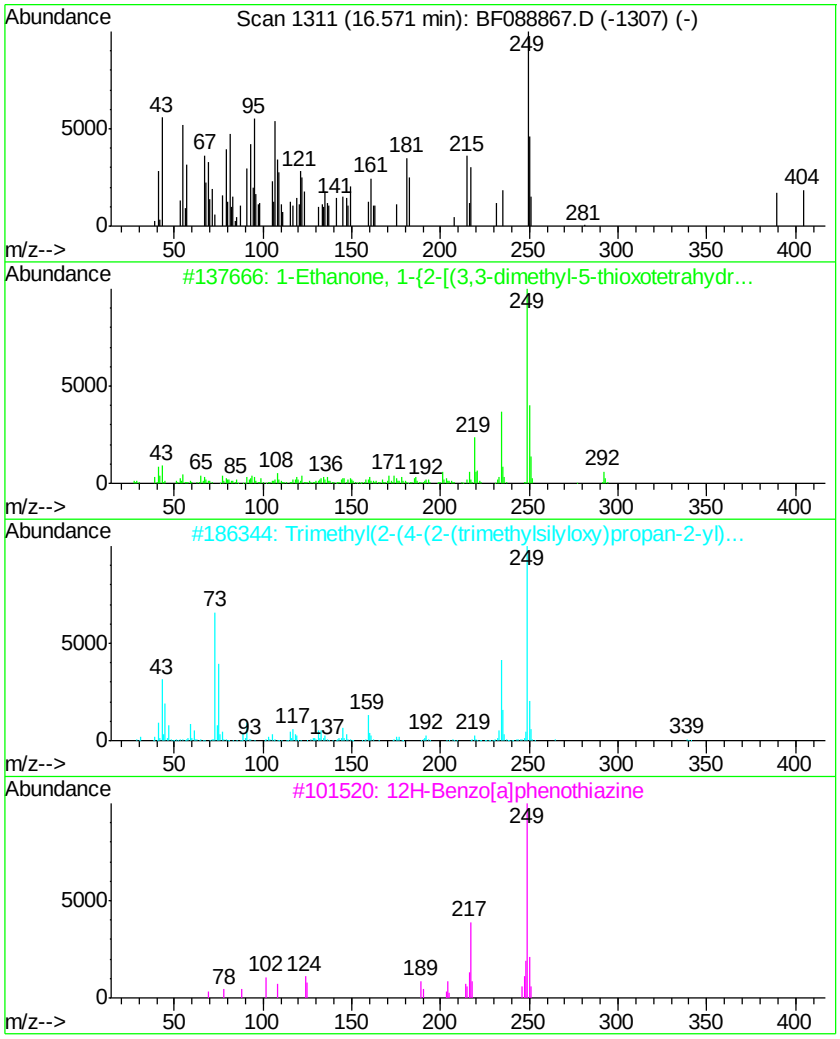
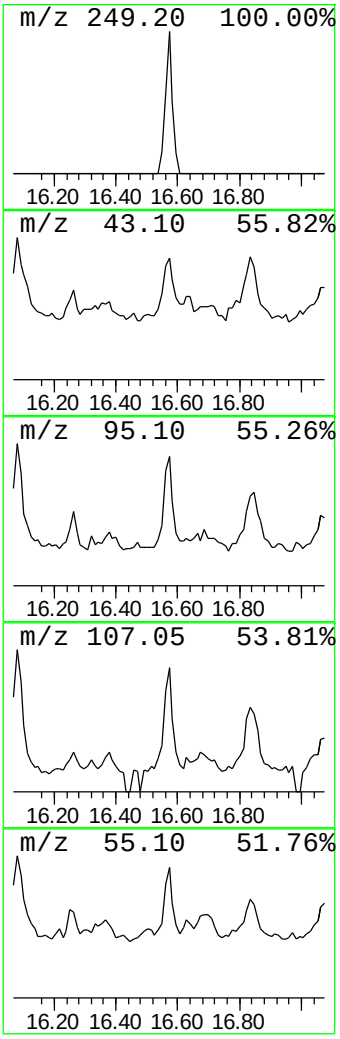
Peak Number 14 unknown16.57 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	3.95 ng	91509	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethanone, 1-{2-[(3,3-dimethyl-...	292	C16H24N2OS	077109-20-7	43
2	Trimethyl(2-(4-(2-(trimethylsily...	354	C18H34O3Si2	1000368-53-8	27
3	12H-Benzo[a]phenothiazine	249	C16H11NS	000225-83-2	25
4	1,3,5-Triazine-2,4-diamine, 6-(c...	249	C11H12ClN5	1000338-25-4	25
5	Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	22





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Operator : UM/SJ
Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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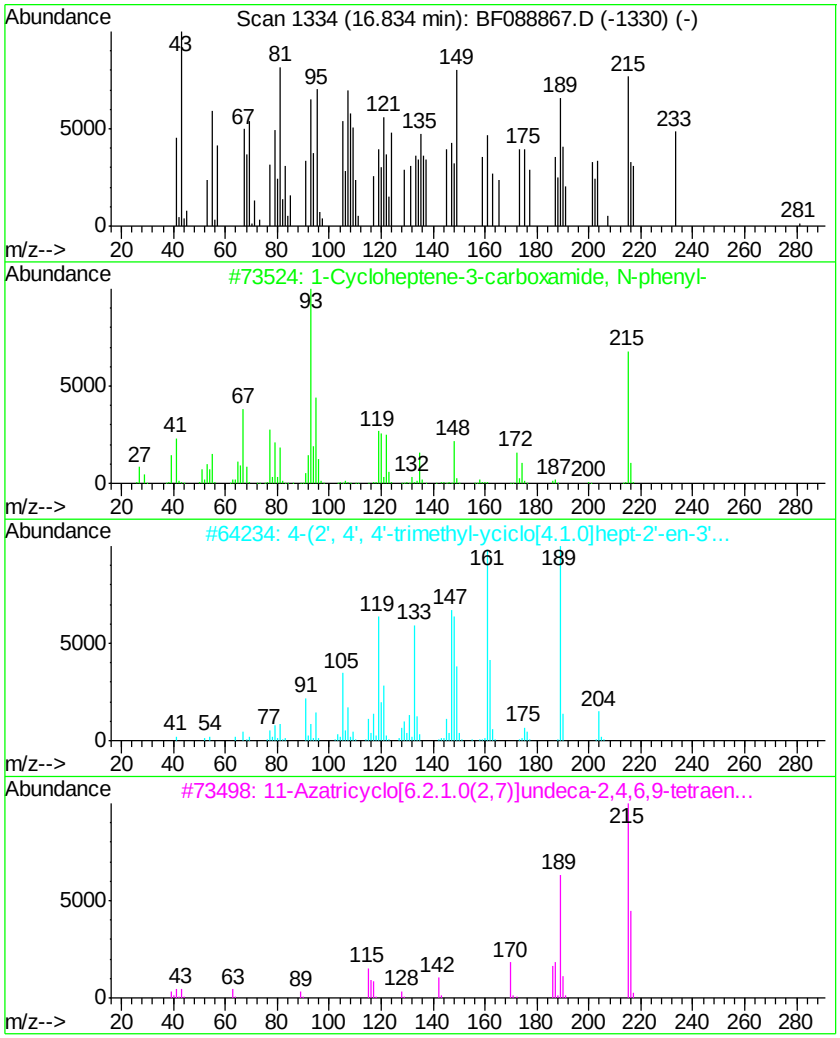
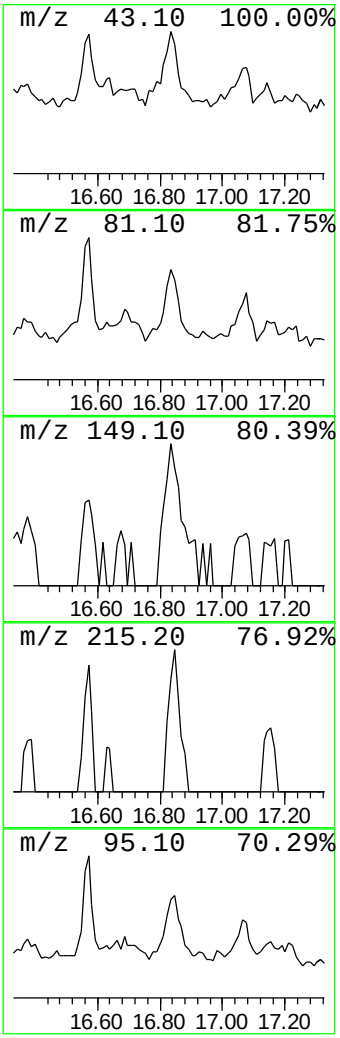
Peak Number 15 unknown16.83 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	5.37 ng	124566	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cycloheptene-3-carboxamide, N-...	215	C14H17NO	1000159-24-4	15
2	4-(2', 4', 4'-trimethyl-ycicloſ4...	204	C14H20O	1000373-94-4	10
3	11-Azatricyclo[6.2.1.0(2,7)]unde...	215	C13H13NO2	1000306-00-6	10
4	.gamma.-Neoclovene	204	C15H24	1000156-11-7	10
5	6-Methyl-2-phenoxymethyl-4-pyrim...	215	C12H13N3O	067386-50-9	10





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Sample : H3813-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-WW002-01

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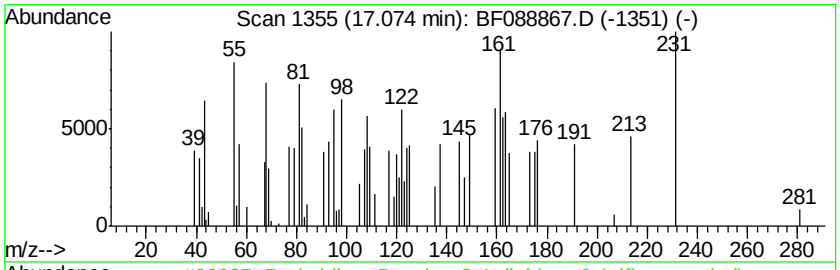
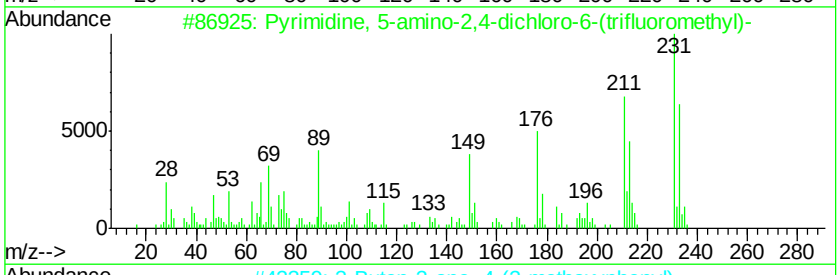
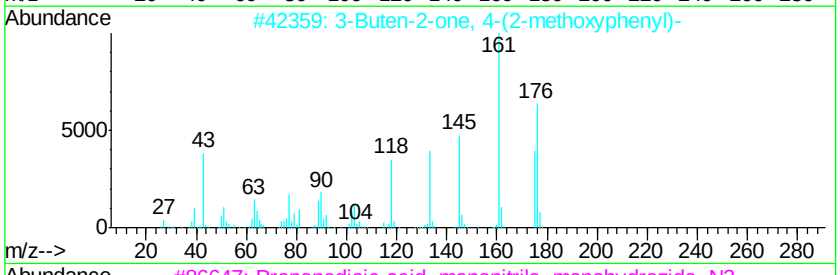
Peak Number 16 unknown17.07 Concentration Rank 16

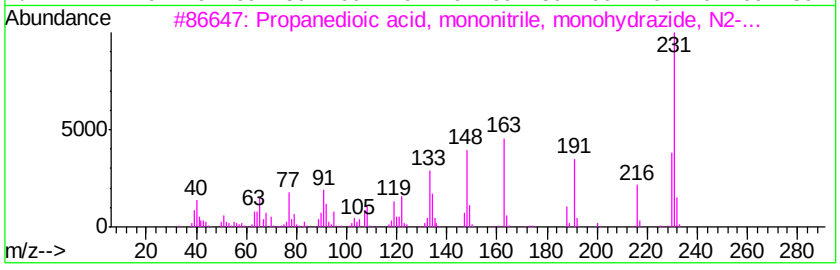
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.07	2.39 ng	55393	Perylene-d12	15.22

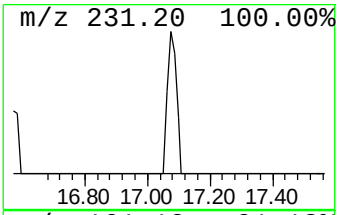
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine, 5-amino-2,4-dichloro...	231	C5H2Cl2F3N3	002925-96-4	27
2	3-Buten-2-one, 4-(2-methoxyphenyl)-	176	C11H12O2	010542-87-7	22
3	Propanedioic acid, mononitrile, ...	231	C12H13N3O2	004980-37-4	22
4	Palladium, bis[(1,2,3-.eta.)-2-m...	216	C8H14Pd	041348-25-8	10
5	Isolongifolene-5-ol	220	C15H24O	1000159-37-0	10

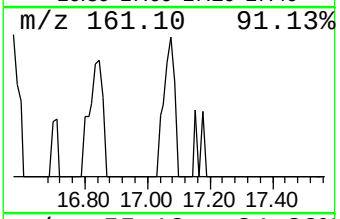


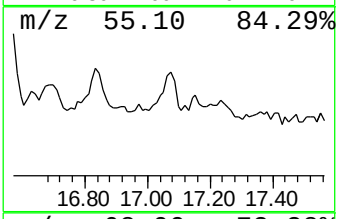


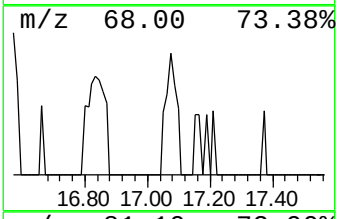


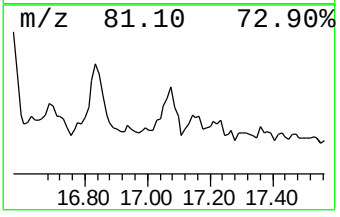












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	5.3	ng	135445	1	6.72	505880	20.0
unknown6.48	6.48	53.9	ng	1362590	1	6.72	505880	20.0
n-Hexadecanoic acid	11.78	14.1	ng	574043	4	11.23	817391	20.0
Octadecanoic acid	12.57	30.0	ng	1040660	5	13.85	693052	20.0
Diethylene glycol...	13.73	8.2	ng	285473	5	13.85	693052	20.0
unknown13.95	13.95	2.7	ng	92905	5	13.85	693052	20.0
Squalene	14.71	3.3	ng	76528	6	15.22	463560	20.0
Cholestan-3-ol, (...	15.86	21.1	ng	488549	6	15.22	463560	20.0
Cholestan-3-one	16.03	13.6	ng	315499	6	15.22	463560	20.0
Cholestan-3-ol	16.08	5.0	ng	115606	6	15.22	463560	20.0
unknown16.57	16.57	4.0	ng	91509	6	15.22	463560	20.0
unknown16.83	16.83	5.4	ng	124566	6	15.22	463560	20.0
unknown17.07	17.07	2.4	ng	55393	6	15.22	463560	20.0