LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

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-BF102116.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	4.956	249	251	255	rBV	420575	511897	20.30%	1.591%
2	5.058	255	260	275	rVB	44575	219936	8.72%	0.683%
3	5.390	287	289	292	rBV	2145950	2127687	84.36%	6.612%
4	6.430	378	380	383	rBV	1507792	2157948	85.56%	6.706%
5	6.567	389	392	394	rBV	2264376	2512727	99.63%	7.809%
6	6.796	410	412	418	rBV	1380247	1279885	50.75%	3.977%
7	6.956	423	426	428	rBV	1827750	1907832	75.64%	5.929%
8	7.367	459	462	464	rBV	857996	1275491	50.57%	3.964%
9	7.470	470	471	478	rVB	33607	43354	1.72%	0.135%
10	8.087	522	525	527	rBV	1925843	1748907	69.34%	5.435%
11	9.162	617	619	622	rBV	2818320	2522167	100.00%	7.838%
12	9.562	652	654	656	rBV	688759	593003	23.51%	1.843%
13	9.836	676	678	681	rBV	1683912	1758990	69.74%	5.466%
14	10.282	715	717	718	rVB	54801	49084	1.95%	0.153%
15	10.499	733	736	739	rBV	27295	46235	1.83%	0.144%
16	10.625	745	747	750	rBV	1362418	1326964	52.61%	4.124%
17	10.750	757	758	762	rVB	95470	106821	4.24%	0.332%
18	10.990	777	779	782	rVB4	21743	33311	1.32%	0.104%
19	11.196	796	797	799	rBV2	48265	51112	2.03%	0.159%
20	11.322	806	808	813	rBV	1599805	1622152	64.32%	5.041%
21	11.391	813	814	817	rVB2	46586	56420	2.24%	0.175%
22	11.551	826	828	833	rBV4	30804	61054	2.42%	0.190%
23	11.631	833	835	840	rVB2	22267	42011	1.67%	0.131%
24	11.722	841	843	846	rVB3	29588	42901	1.70%	0.133%
25	11.825	850	852	853	rBV	29988	31035	1.23%	0.096%
26	11.859	853	855	856	rVV	34176	41890	1.66%	0.130%
27	11.939	860	862	866	rVB2	31086	58384	2.31%	0.181%
28	12.031	866	870	876	rBV3	23843	61113	2.42%	0.190%
29	12.145	876	880	882	rVB3	22325	58183	2.31%	0.181%
30	12.373	898	900	901	rBV	43193	46795	1.86%	0.145%
31	12.419	902	904	906	rVB2	28984	45069	1.79%	0.140%
32	12.465	906	908	911	rBV2	53820	87428	3.47%	0.272%
33	12.522	911	913	917	rVV2	429132	663495	26.31%	2.062%
34	12.762	930	934	935	rBV	238888	287443	11.40%	0.893%

LSC Area Percent Report

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Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

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-BF102116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.796	935	937	945	rVV	1085763	1458013	57.81%	4.531%
36	12.911	945	947	951	rVV	2067884	1911057	75.77%	5.939%
37	12.979	951	953	957	rVB2	29023	68437	2.71%	0.213%
38	13.151	965	968	970	rBV3	31104	60437	2.40%	0.188%
39	13.196	970	972	976	rBV2	37591	61456	2.44%	0.191%
40	13.322	981	983	986	rVV2	19065	27822	1.10%	0.086%
41	13.368	986	987	990	rVB3	35467	48017	1.90%	0.149%
42	13.608	1006	1008	1011	rVB2	42919	56068	2.22%	0.174%
43	13.711	1015	1017	1018	rBV2	28556	34871	1.38%	0.108%
44	13.814	1024	1026	1031	rBV2	210483	294713	11.68%	0.916%
45	13.962	1036	1039	1045	rBV	1105296	1339007	53.09%	4.161%
46	14.065	1046	1048	1050	rBV2	29800	35704	1.42%	0.111%
47	14.454	1079	1082	1084	rBV	144283	229962	9.12%	0.715%
48	14.877	1117	1119	1123	rVB3	40312	63106	2.50%	0.196%
49	14.979	1125	1128	1133	rBV	155950	299151	11.86%	0.930%
50	15.059	1133	1135	1140	rVV2	96132	212617	8.43%	0.661%
51	15.265	1151	1153	1156	rVB	92829	113995	4.52%	0.354%
52	15.322	1156	1158	1161	rBV	91920	135518	5.37%	0.421%
53	15.379	1161	1163	1166	rBV	668880	984155	39.02%	3.058%
54	15.608	1181	1183	1186	rVB2	53686	75062	2.98%	0.233%
55	15.837	1200	1203	1205	rBV	179133	286925	11.38%	0.892%
56	15.882	1205	1207	1212	rVV3	58068	123595	4.90%	0.384%
57	15.974	1213	1215	1217	rVB2	48121	68948	2.73%	0.214%
58	16.751	1281	1283	1290	rVB2	46552	104532	4.14%	0.325%
59	17.163	1316	1319	1325	rBV	45534	126545	5.02%	0.393%
60	17.300	1328	1331	1335	rBV4	52113	142466	5.65%	0.443%
61	18.260	1412	1415	1421	rVB7	37712	97407	3.86%	0.303%
62	19.231	1496	1500	1512	rVB7	52641	240658	9.54%	0.748%

Sum of corrected areas: 32178968

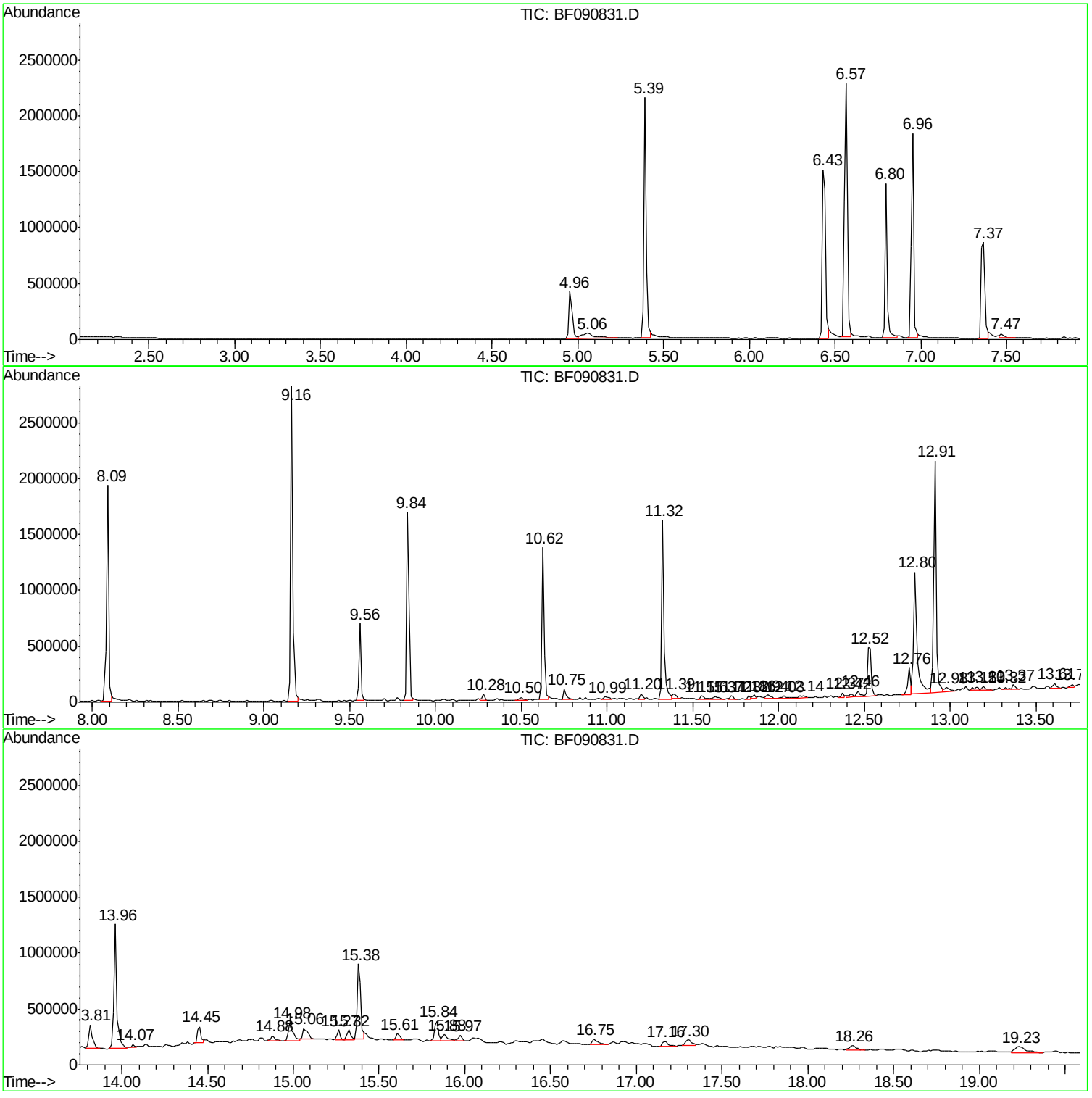
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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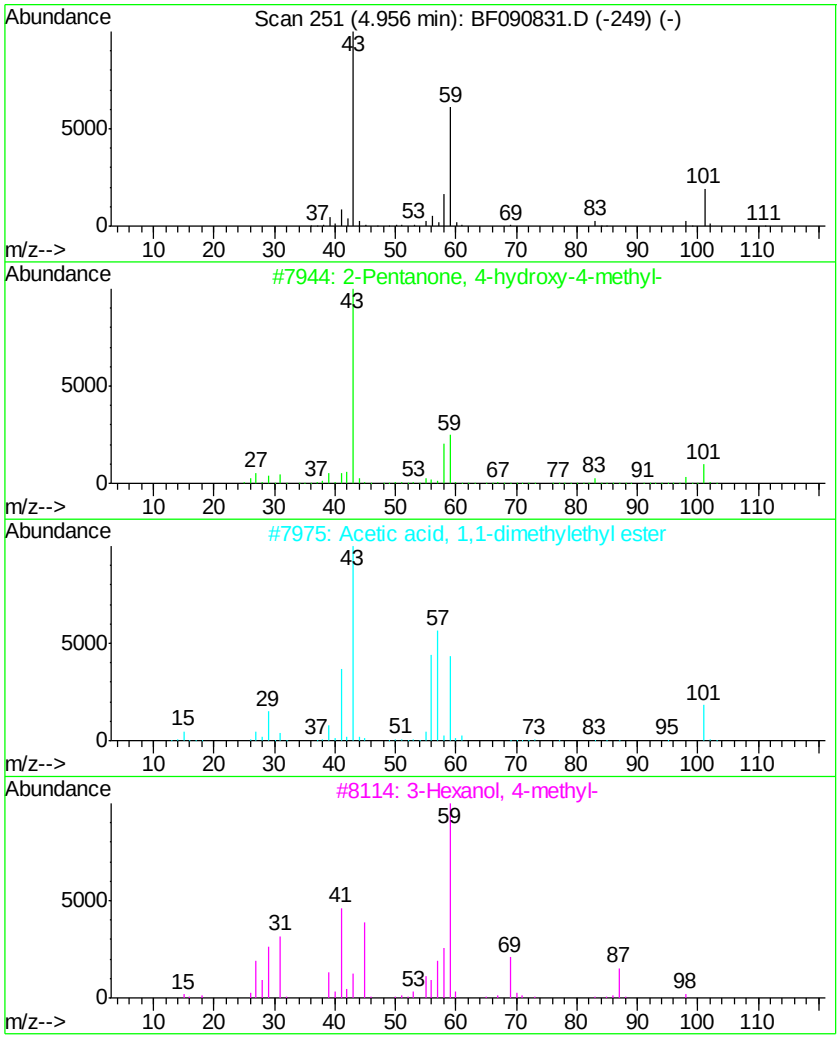
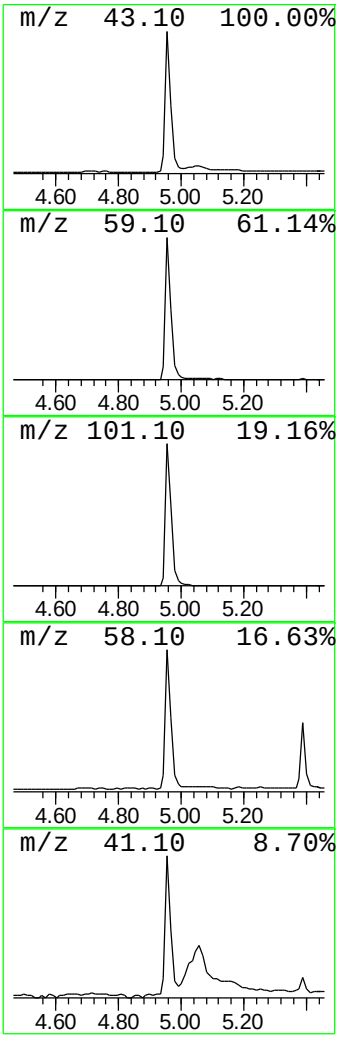
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.00 ng	511897	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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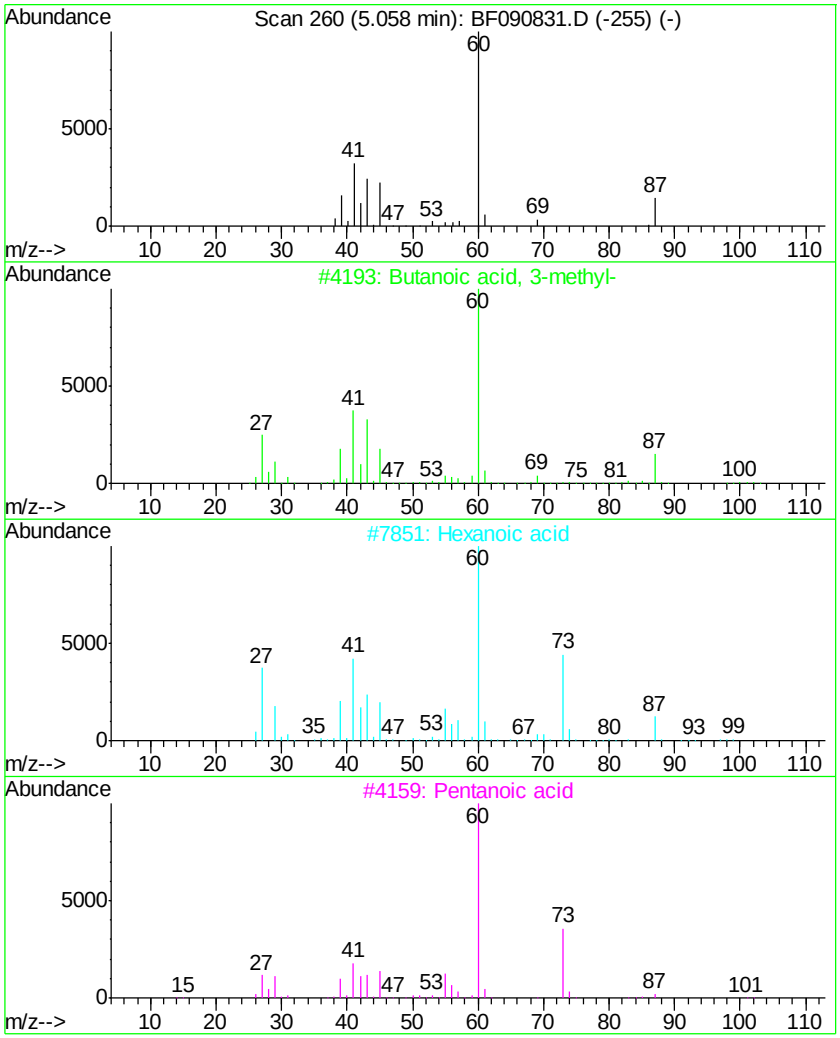
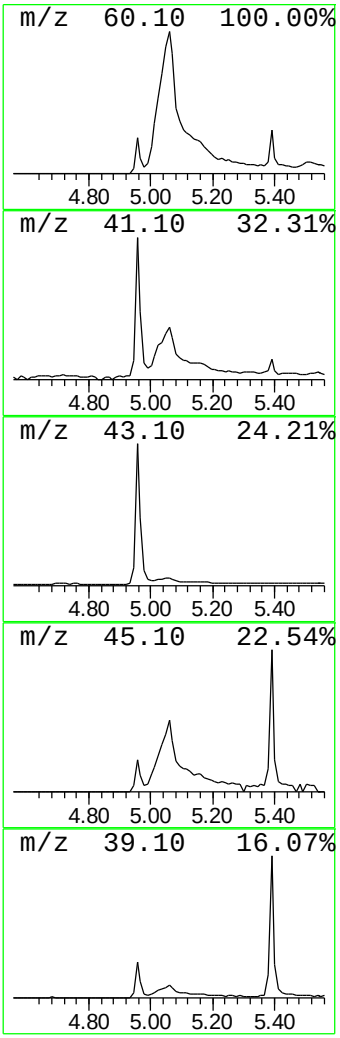
Peak Number 2 unknown5.06 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.44 ng	219936	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	40
2	Hexanoic acid	116	C6H12O2	000142-62-1	9
3	Pentanoic acid	102	C5H10O2	000109-52-4	9
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
5	Urea	60	CH4N2O	000057-13-6	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
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Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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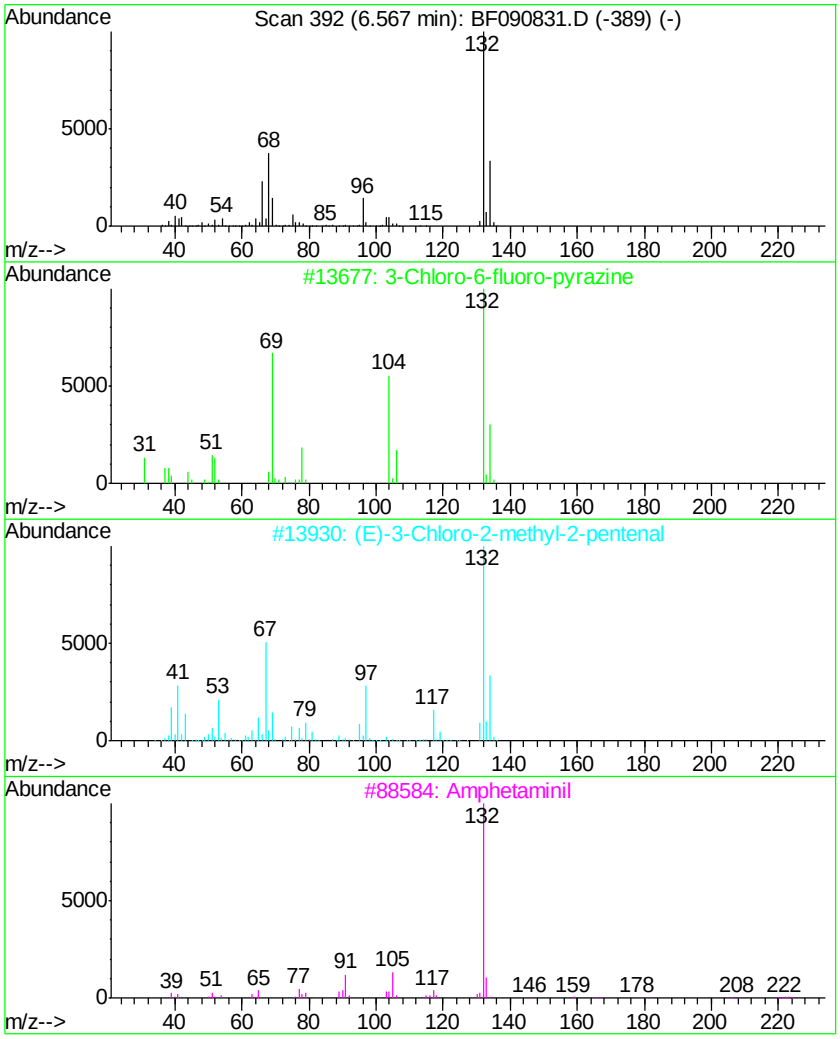
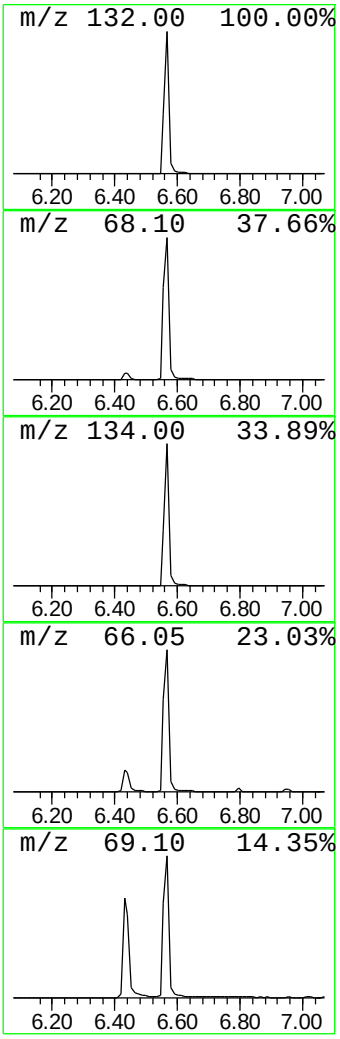
Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	39.26 ng	2512730	1,4-Dichlorobenzene-d4	6.80

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	Amphetaminil	250	C17H18N2	017590-01-1	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
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Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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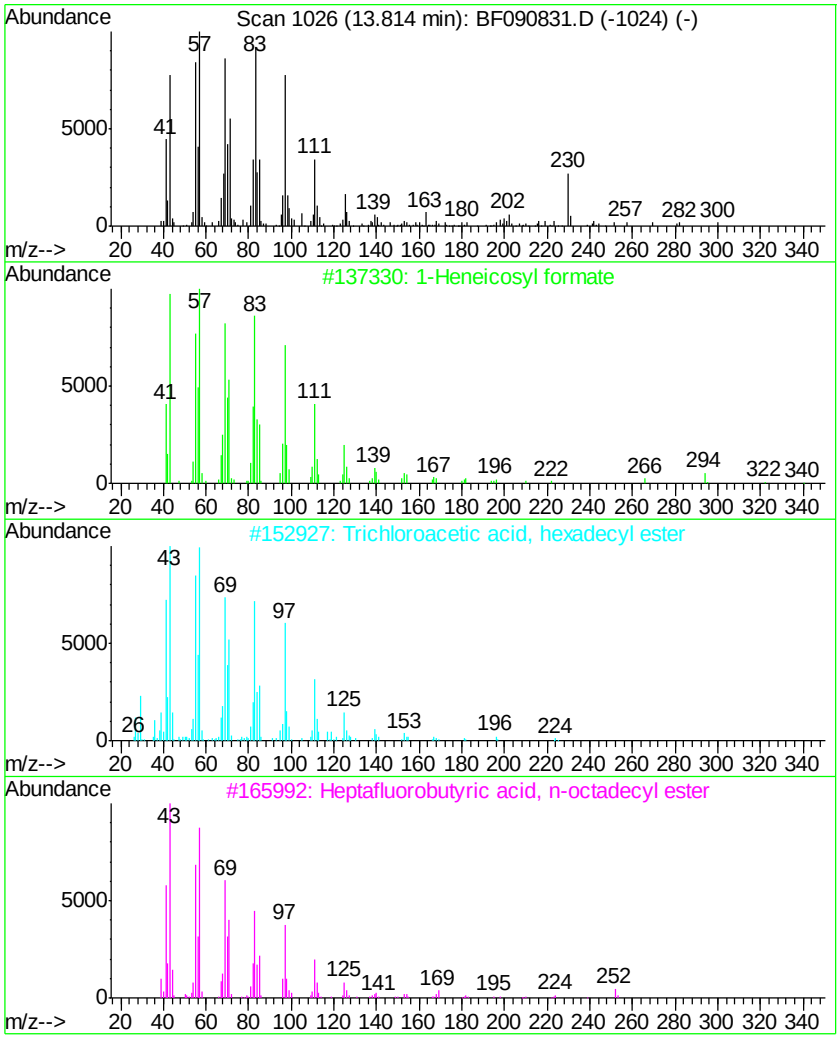
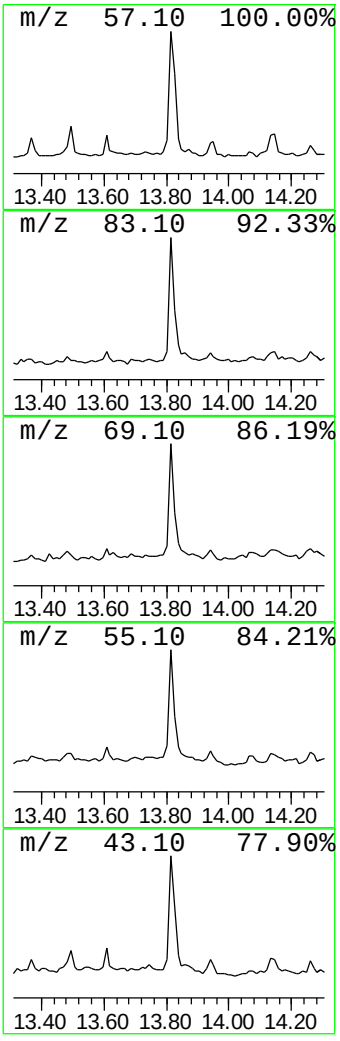
Peak Number 5 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.40 ng	294713	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	1-Tetracosanol	354	C24H50O	000506-51-4	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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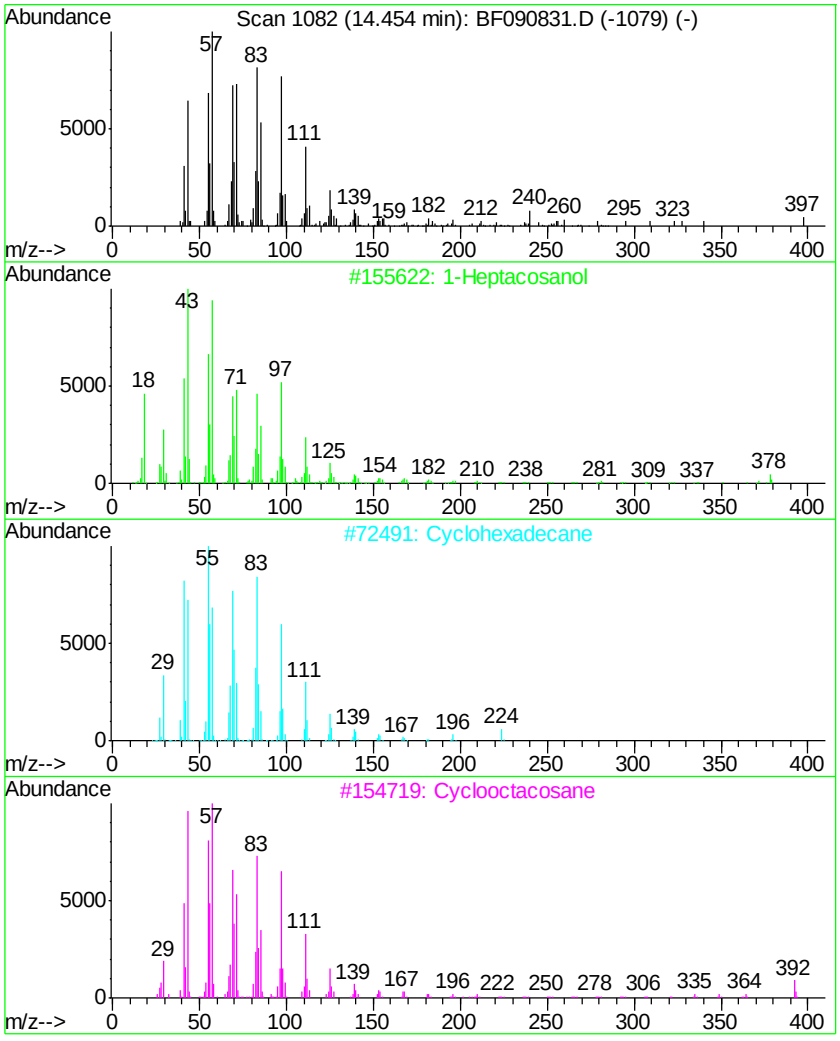
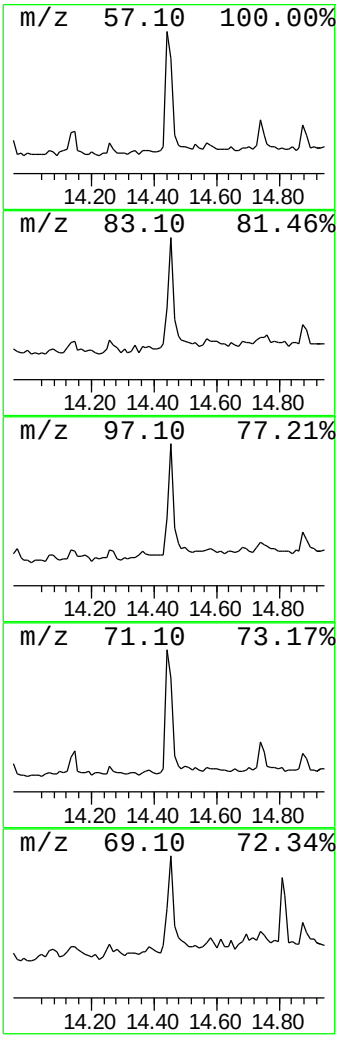
Peak Number 6 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.43 ng	229962	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Cyclohexadecane	224	C16H32	000295-65-8	87
3	Cyclooctacosane	392	C28H56	000297-24-5	81
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	74
5	Cyclotetracosane	336	C24H48	000297-03-0	70





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Sample : H5396-04 2X
Misc :
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Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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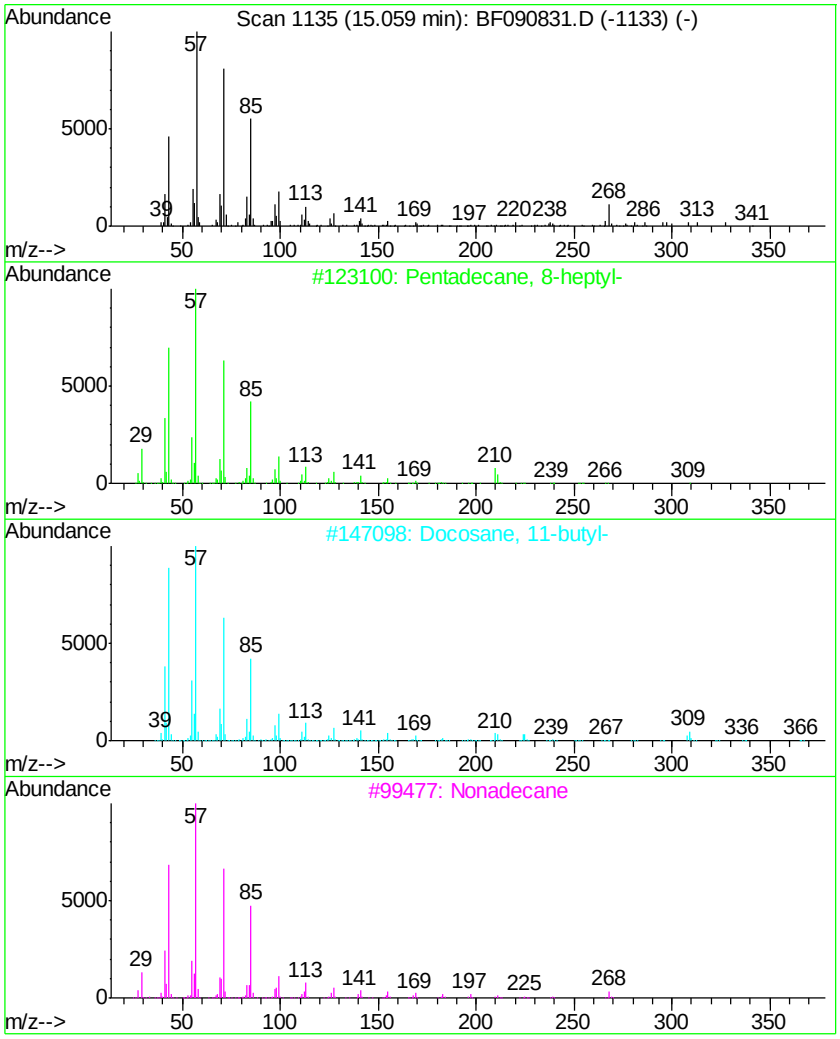
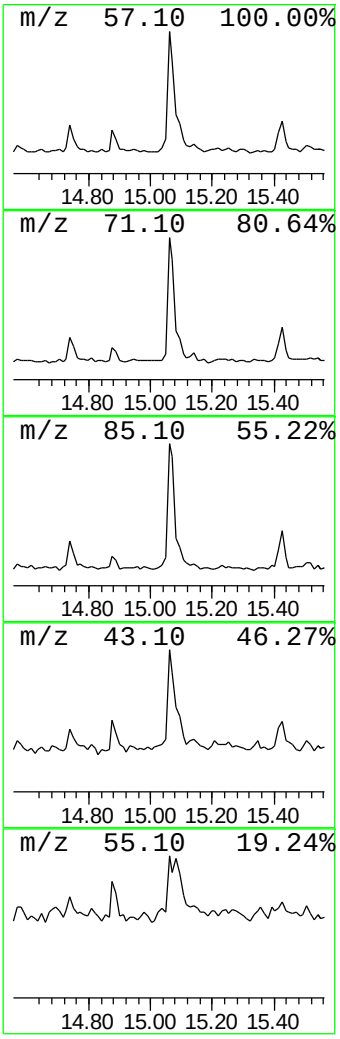
Peak Number 7 Pentadecane, 8-heptyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	4.32 ng	212617	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Pentacosane	352	C25H52	000629-99-2	80





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Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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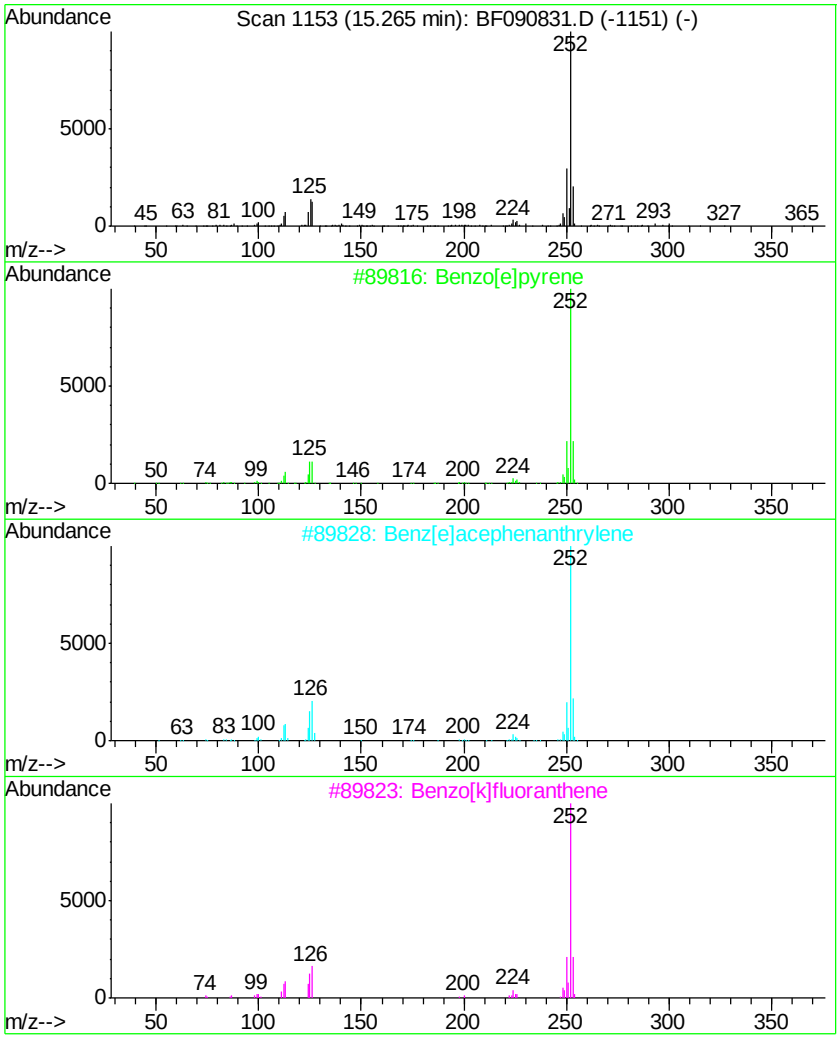
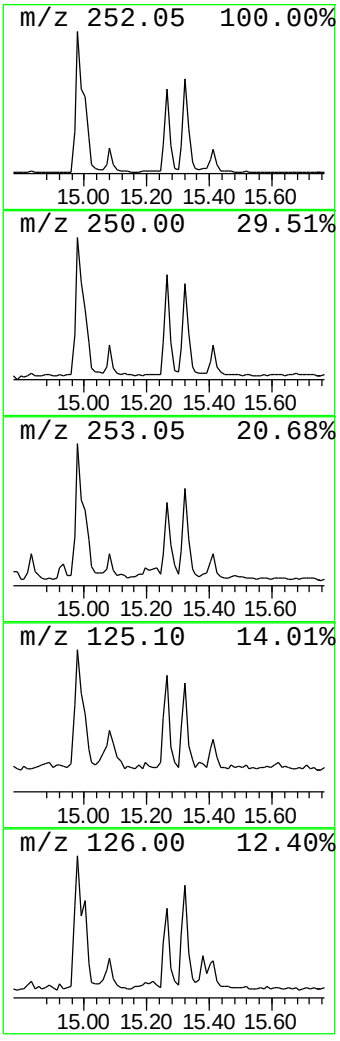
Peak Number 8 Benzo[e]pyrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.32 ng	113995	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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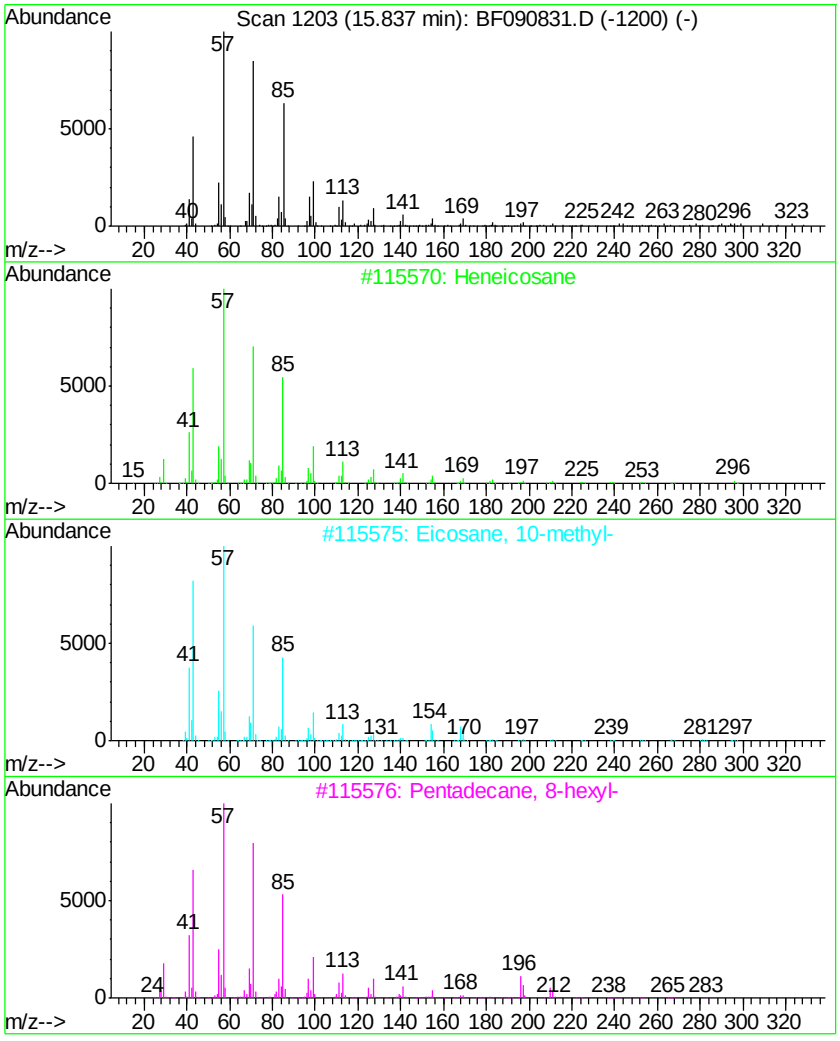
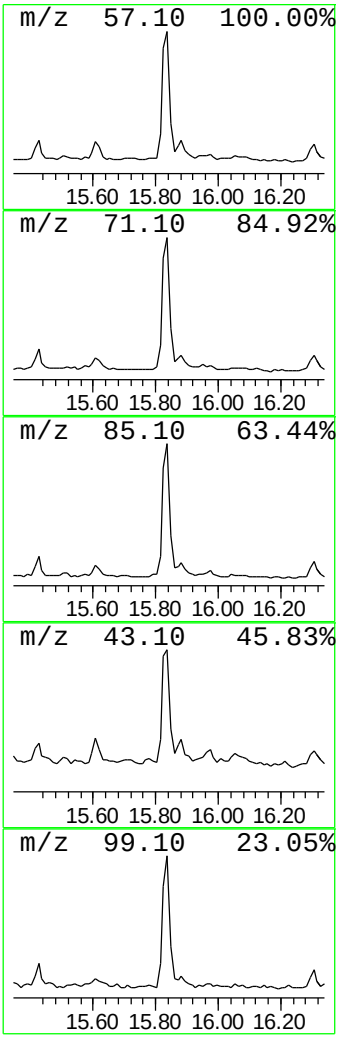
Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	5.83 ng	286925	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	92
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
4	Tetratriacontane	479	C34H70	014167-59-0	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





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Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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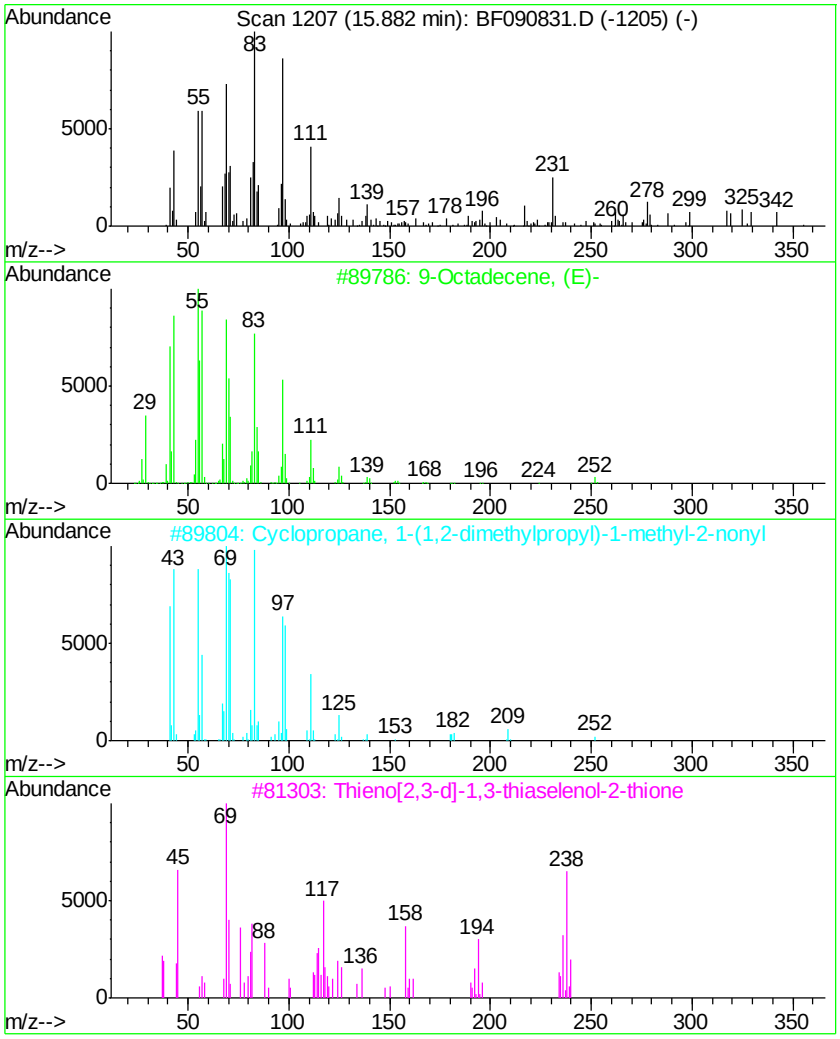
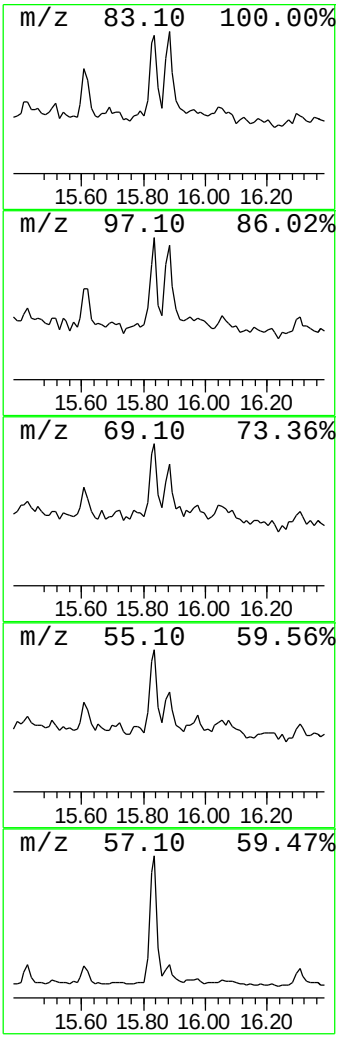
Peak Number 11 9-Octadecene, (E)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.51 ng	123595	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	72
2	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	72
3	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
4	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	53
5	Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	054889-87-1	46





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Sample : H5396-04 2X
Misc :
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Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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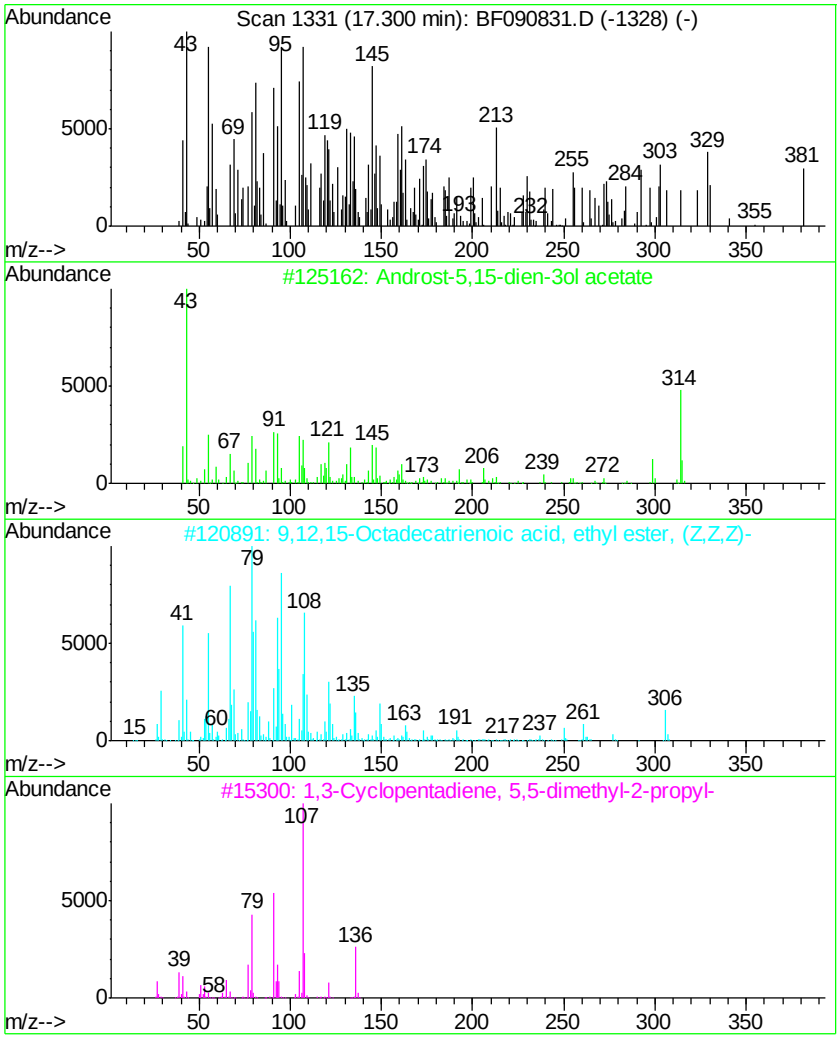
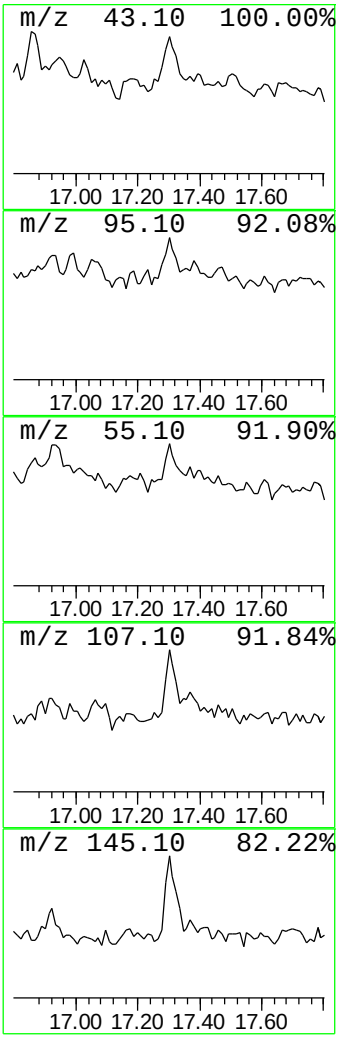
Peak Number 14 unknown17.30 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.90 ng	142466	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Androst-5,15-dien-3ol acetate	314	C21H30O2	1000251-88-0	27
2	9,12,15-Octadecatrienoic acid, e...	306	C20H34O2	001191-41-9	15
3	1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-0	15
4	Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	001196-01-6	11
5	Arsonous dichloride, methyl-	160	CH3AsCl2	000593-89-5	11





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Data File : BF090831.D
Acq On : 26 Oct 2016 2:05
Operator : UM/SJ
Sample : H5396-04 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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TIC Integration Parameters: LSCINT.P

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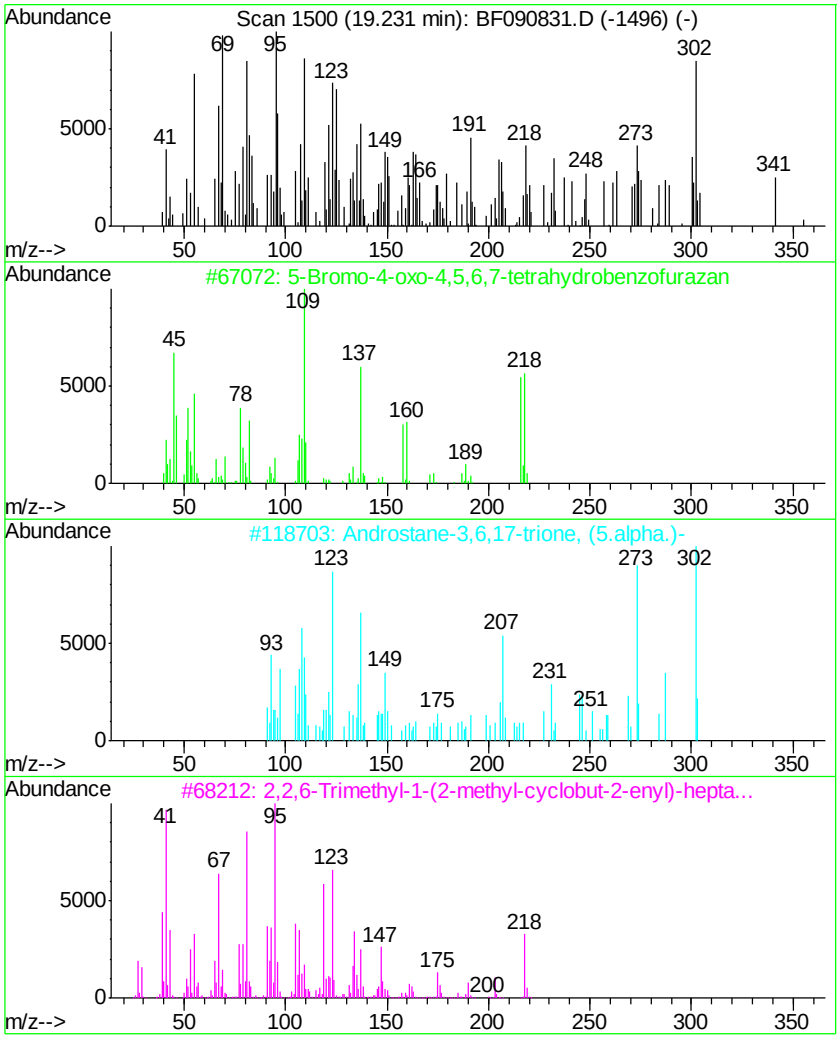
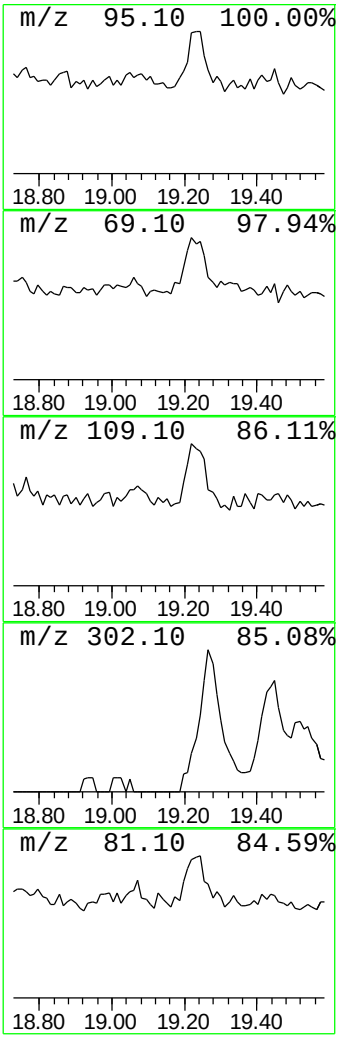
Peak Number 15 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	4.89 ng	240658	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
2	Androstane-3,6,17-trione, (5.alp...	302	C19H26O3	002243-05-2	43
3	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
4	Androstane-3,6,17-trione, (5.bet...	302	C19H26O3	026991-58-2	30
5	Androstan-3,17-dione, 9,11-epoxy-	302	C19H26O3	1000128-33-8	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102516\
Data File : BF090831.D
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Operator : UM/SJ
Sample : H5396-04 2X
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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P2-S3

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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...	4.96	8.0	ng	511897	1	6.80	1279890	20.0
unknown5.06	5.06	3.4	ng	219936	1	6.80	1279890	20.0
unknown6.57	6.57	39.3	ng	2512730	1	6.80	1279890	20.0
1-Heneicosyl formate	13.81	4.4	ng	294713	5	13.96	1339010	20.0
1-Heptacosanol	14.45	3.4	ng	229962	5	13.96	1339010	20.0
Pentadecane, 8-he...	15.06	4.3	ng	212617	6	15.38	984155	20.0
Benzo[e]pyrene	15.27	2.3	ng	113995	6	15.38	984155	20.0
Heneicosane	15.84	5.8	ng	286925	6	15.38	984155	20.0
9-Octadecene, (E)-	15.88	2.5	ng	123595	6	15.38	984155	20.0
unknown17.30	17.30	2.9	ng	142466	6	15.38	984155	20.0
5-Bromo-4-oxo-4,5...	19.23	4.9	ng	240658	6	15.38	984155	20.0