LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090826.D
Acq On : 25 Oct 2016 23:50
Operator : UM/SJ
Sample : H5394-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

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	4.967	249	252	261	rBV	482591	738497	15.36%	1.550%
2	5.401	287	290	292	rBV	3634798	4269033	88.81%	8.957%
3	6.441	378	381	383	rBV	3183014	3647799	75.88%	7.654%
4	6.567	389	392	394	rBV	3865334	3908335	81.30%	8.201%
5	6.796	410	412	423	rBV	952802	951246	19.79%	1.996%
6	6.956	423	426	428	rBV	3245827	3218562	66.96%	6.753%
7	7.367	459	462	464	rBV	2156153	2438076	50.72%	5.116%
8	7.470	469	471	478	rVB	26960	64395	1.34%	0.135%
9	8.087	522	525	527	rBV	1210346	1279992	26.63%	2.686%
10	9.162	617	619	622	rBV	4161812	4807014	100.00%	10.086%
11	9.253	625	627	629	rVB	50601	55355	1.15%	0.116%
12	9.562	652	654	656	rBV	1463757	1255205	26.11%	2.634%
13	9.779	671	673	676	rBV	95193	68372	1.42%	0.143%
14	9.836	676	678	680	rVV	1625186	1498984	31.18%	3.145%
15	10.248	712	714	716	rBV	209446	255148	5.31%	0.535%
16	10.282	716	717	718	rVB	129424	89664	1.87%	0.188%
17	10.499	733	736	739	rBV	68263	94238	1.96%	0.198%
18	10.625	745	747	750	rBV2	2167247	2866988	59.64%	6.016%
19	10.751	756	758	763	rVB	205905	252431	5.25%	0.530%
20	10.945	772	775	779	rBV4	27839	70022	1.46%	0.147%
21	11.196	796	797	799	rBV	114149	118956	2.47%	0.250%
22	11.231	799	800	803	rVB	68137	59620	1.24%	0.125%
23	11.322	806	808	809	rBV	1539181	1367127	28.44%	2.869%
24	11.402	812	815	817	rVB2	60296	105034	2.19%	0.220%
25	11.562	826	829	833	rBV4	52345	118664	2.47%	0.249%
26	11.631	833	835	836	rBV	57164	68125	1.42%	0.143%
27	11.859	853	855	856	rVV	54203	77388	1.61%	0.162%
28	11.939	860	862	867	rVB2	91962	162243	3.38%	0.340%
29	12.031	869	870	874	rVB	64293	59274	1.23%	0.124%
30	12.419	902	904	906	rVV2	64366	110387	2.30%	0.232%
31	12.534	912	914	917	rBV	970366	875533	18.21%	1.837%
32	12.682	924	927	931	rBV3	26844	59295	1.23%	0.124%
33	12.762	931	934	935	rVV	757795	832264	17.31%	1.746%
34	12.796	935	937	943	rVV	572036	790094	16.44%	1.658%

LSC Area Percent Report

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Acq On : 25 Oct 2016 23:50
Operator : UM/SJ
Sample : H5394-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

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	12.911	945	947	950	rVV	3729856	4409212	91.72%	9.252%
36	12.979	951	953	955	rVV2	67903	138759	2.89%	0.291%
37	13.094	959	963	965	rVV	89343	153822	3.20%	0.323%
38	13.162	965	969	970	rVV2	64648	112553	2.34%	0.236%
39	13.196	970	972	976	rVB2	72488	99645	2.07%	0.209%
40	13.402	988	990	995	rVV3	32624	66645	1.39%	0.140%
41	13.494	995	998	1001	rVB4	28752	63704	1.33%	0.134%
42	13.711	1014	1017	1018	rBV	49993	73309	1.53%	0.154%
43	13.757	1018	1021	1024	rVV4	36381	93413	1.94%	0.196%
44	13.814	1024	1026	1031	rVB2	313853	357113	7.43%	0.749%
45	13.962	1035	1039	1046	rBV2	1083224	1744243	36.29%	3.660%
46	14.065	1046	1048	1050	rBV	64349	60439	1.26%	0.127%
47	14.351	1068	1073	1074	rBV	49398	80775	1.68%	0.169%
48	14.454	1078	1082	1085	rBV2	97672	230206	4.79%	0.483%
49	14.808	1111	1113	1118	rBV3	45895	83775	1.74%	0.176%
50	14.979	1125	1128	1133	rBV	266247	523928	10.90%	1.099%
51	15.060	1133	1135	1140	rVV4	68566	171562	3.57%	0.360%
52	15.265	1150	1153	1156	rVB	131592	194985	4.06%	0.409%
53	15.322	1156	1158	1161	rBV	191561	270307	5.62%	0.567%
54	15.380	1161	1163	1169	rVV	723991	957759	19.92%	2.010%
55	15.837	1200	1203	1205	rBV	53695	96225	2.00%	0.202%
56	15.882	1205	1207	1211	rVB2	41692	97633	2.03%	0.205%
57	16.568	1264	1267	1275	rVB4	35589	107797	2.24%	0.226%
58	16.751	1279	1283	1288	rBV2	84431	193908	4.03%	0.407%
59	16.923	1295	1298	1300	rBV	22231	56706	1.18%	0.119%
60	17.151	1315	1318	1327	rBV	80533	221628	4.61%	0.465%
61	17.300	1327	1331	1335	rVV6	34231	105657	2.20%	0.222%
62	17.380	1335	1338	1343	rVB	19992	55551	1.16%	0.117%
63	18.260	1411	1415	1420	rVB4	22006	65705	1.37%	0.138%
64	19.231	1495	1500	1507	rVB7	28303	138441	2.88%	0.290%

Sum of corrected areas: 47658765

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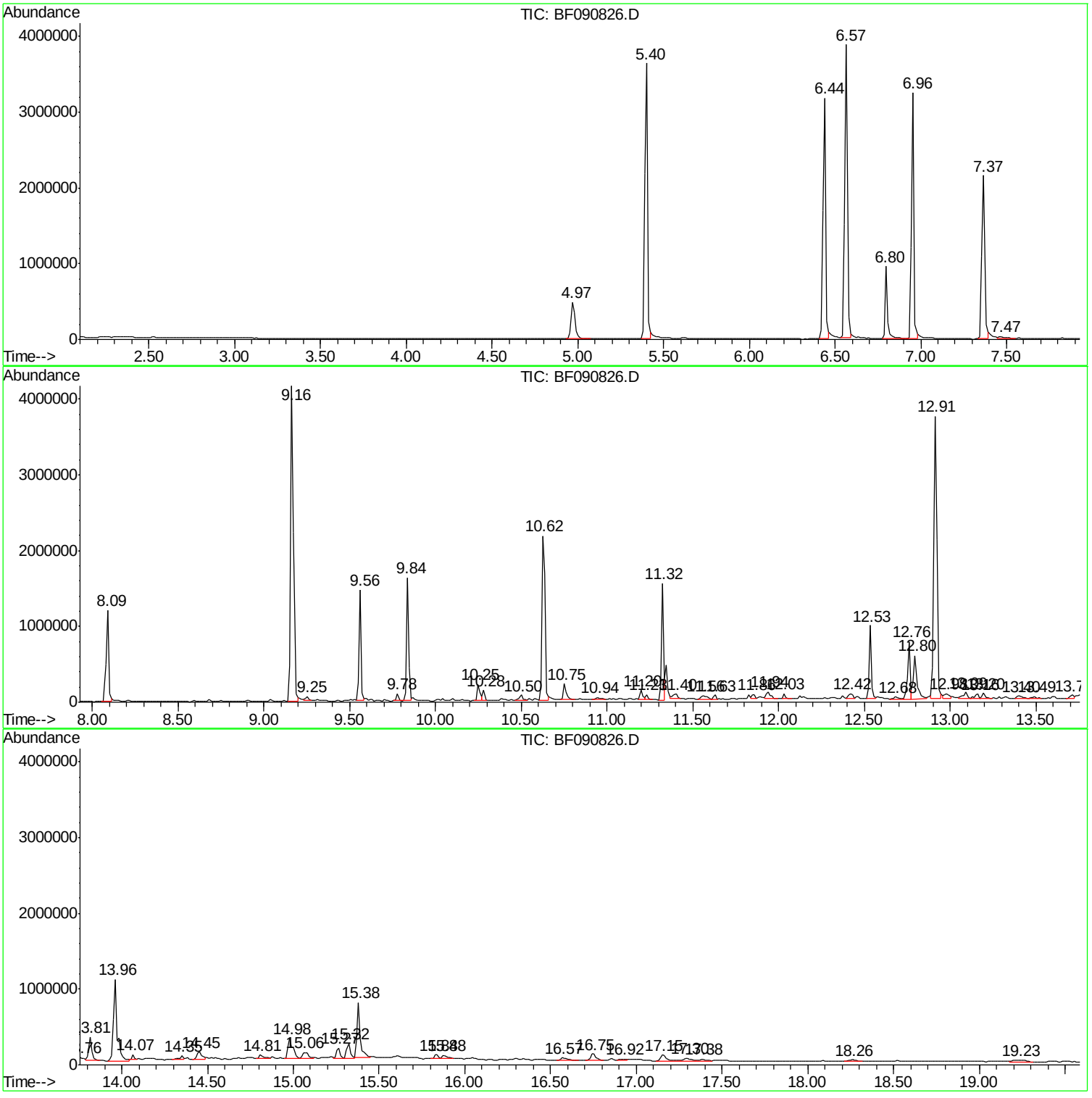
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BOTTOM-CENTER

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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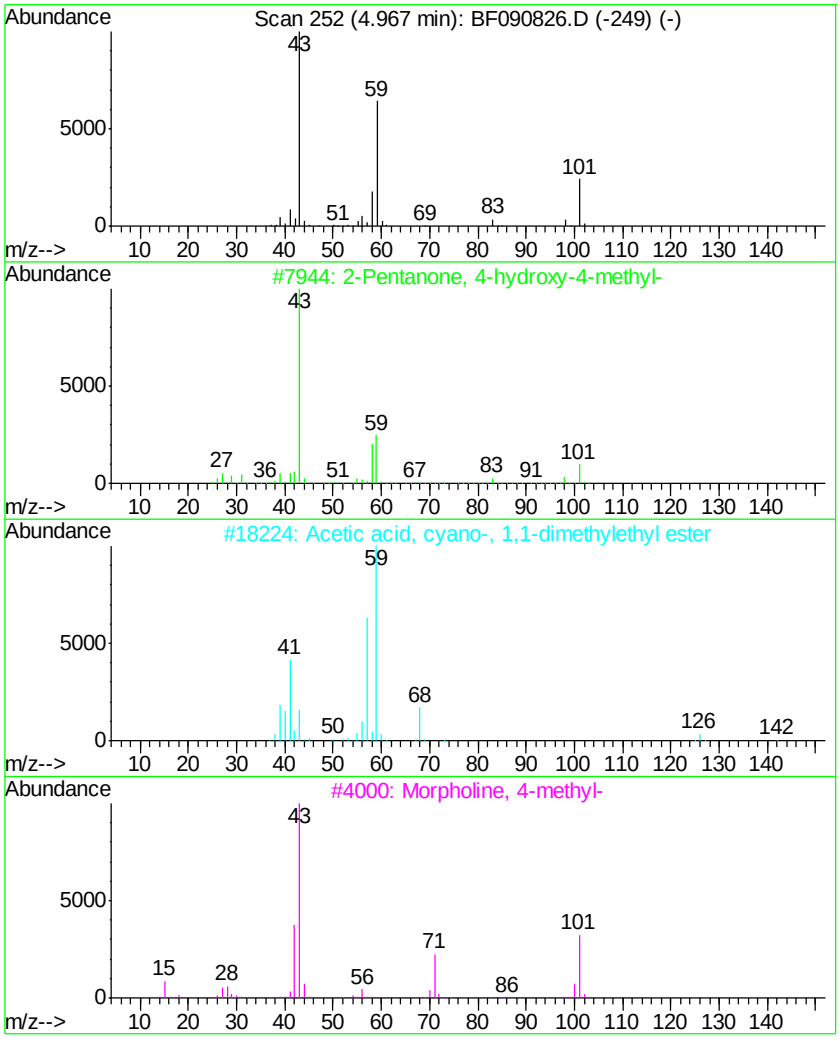
TIC Integration Parameters: LSCINT.P

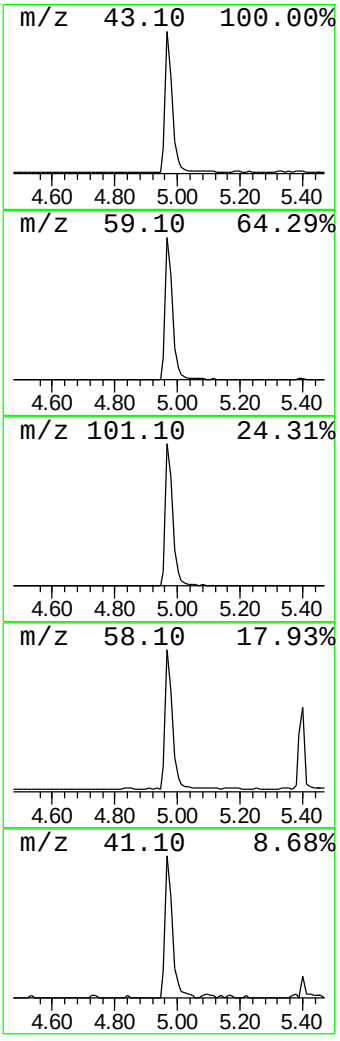
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	15.53 ng	738497	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	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : H5394-06
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Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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TIC Library : C:\DATABASE\NIST02.L
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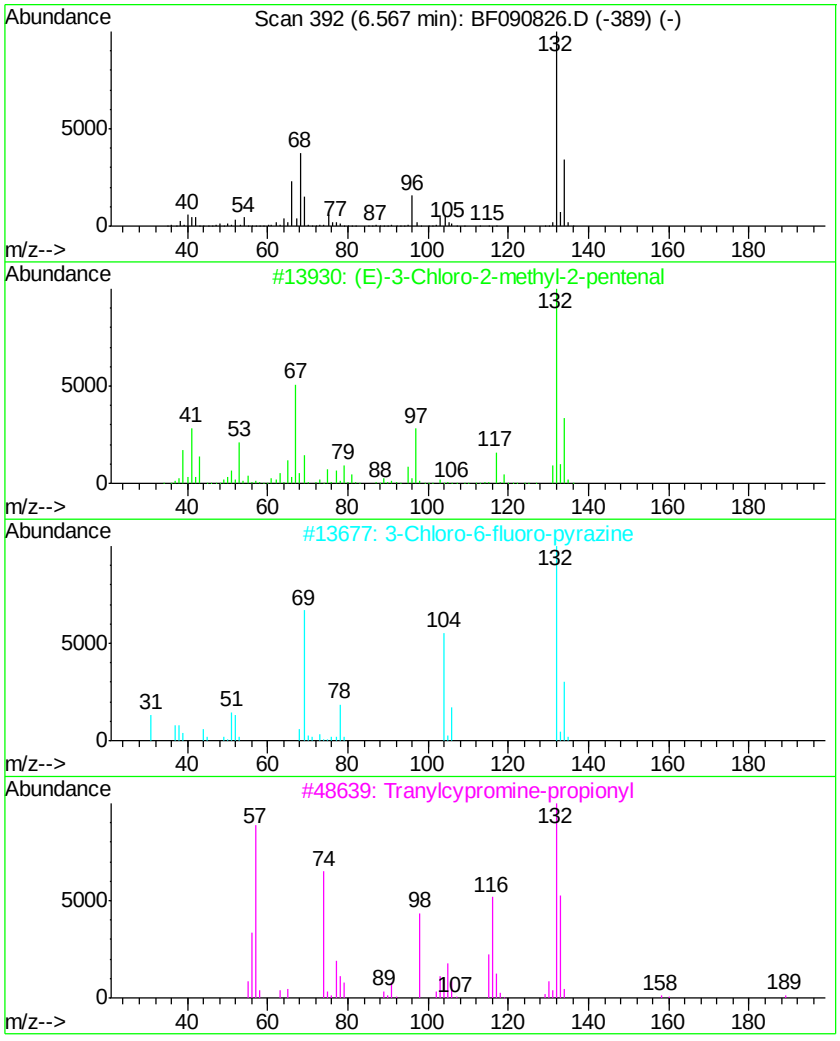
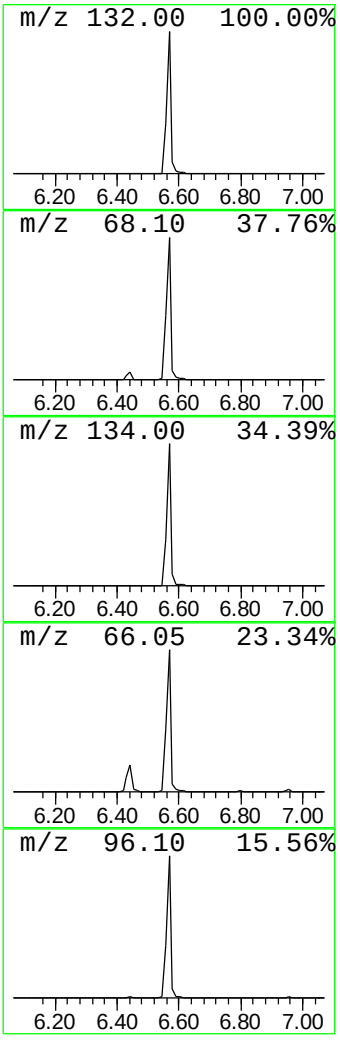
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	82.17 ng	3908340	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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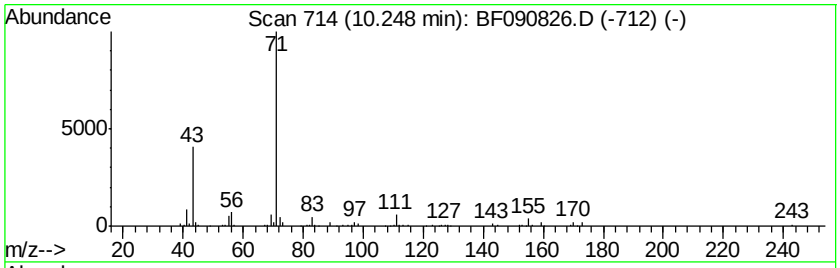
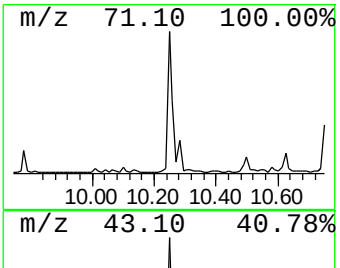
****

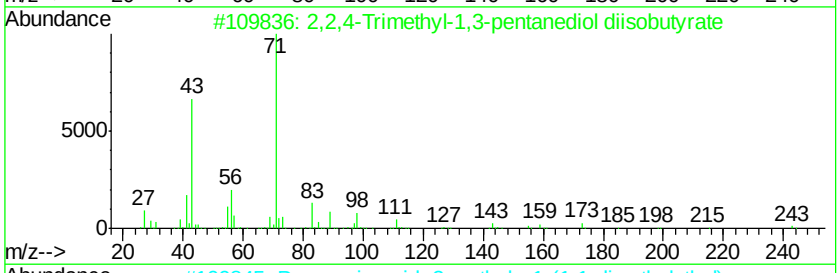
Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 8

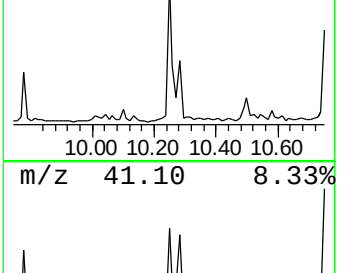
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	3.40 ng	255148	Acenaphthene-d10	9.84

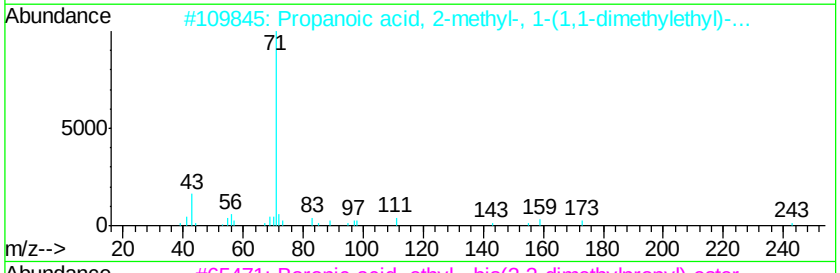
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	72
2	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	56
3	Boronic acid, ethyl-, bis(2,2-di...	214	C12H27BO2	067753-47-3	39
4	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	39
5	3-Methyl-hepta-1,6-dien-3-ol	126	C8H14O	034780-69-3	39

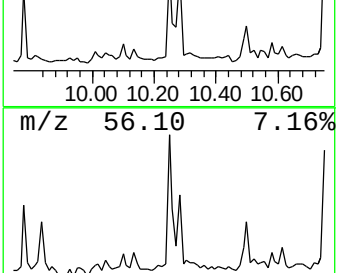


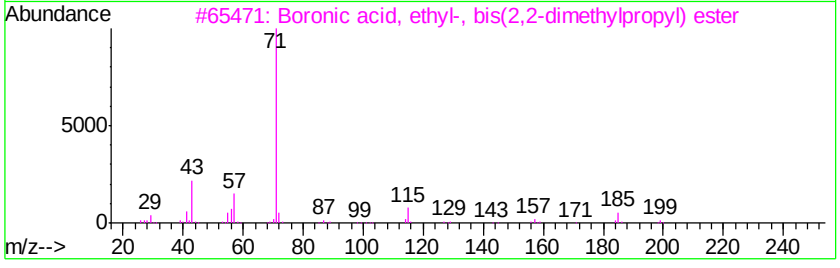


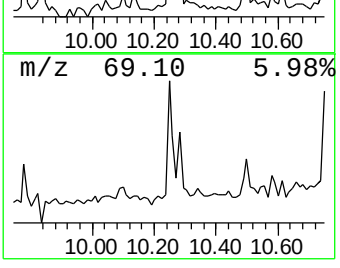












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

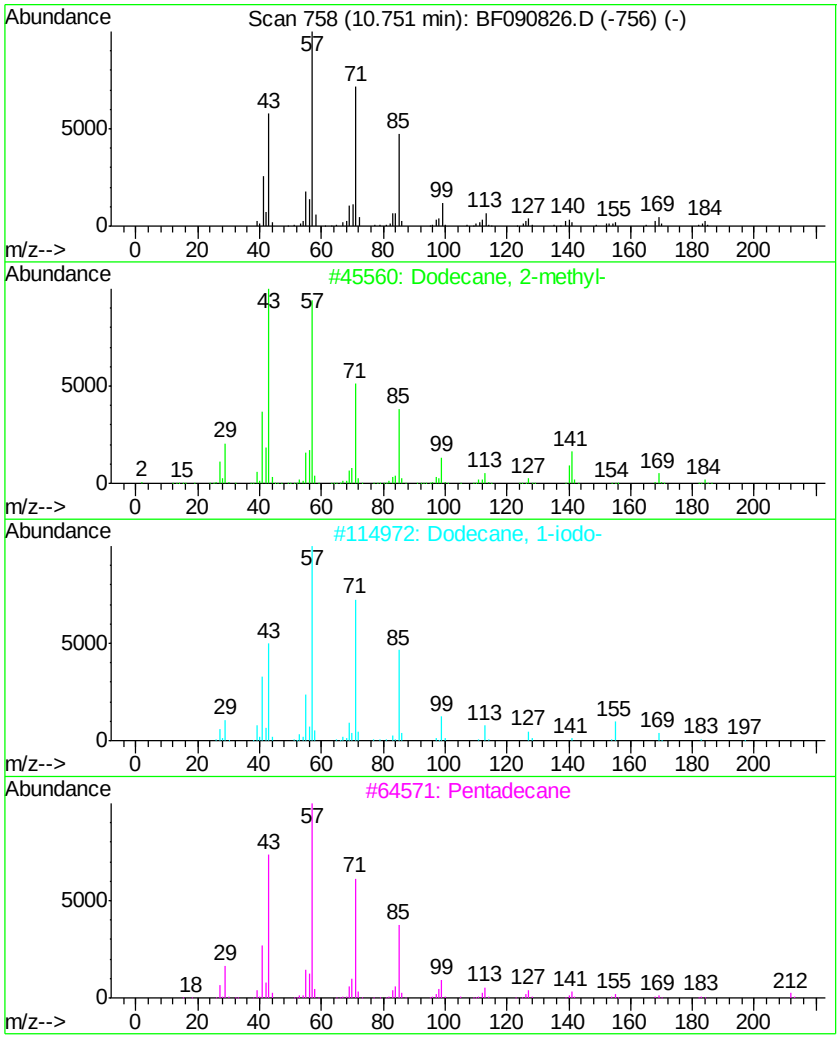
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

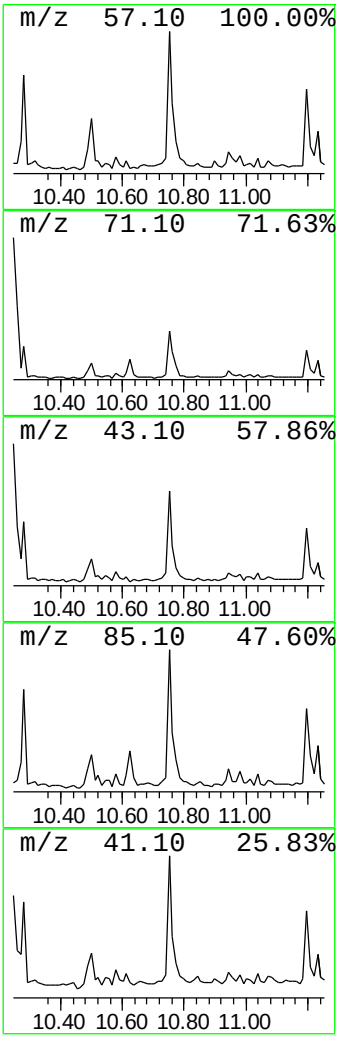
****

Peak Number 5 Dodecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	3.69 ng	252431	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





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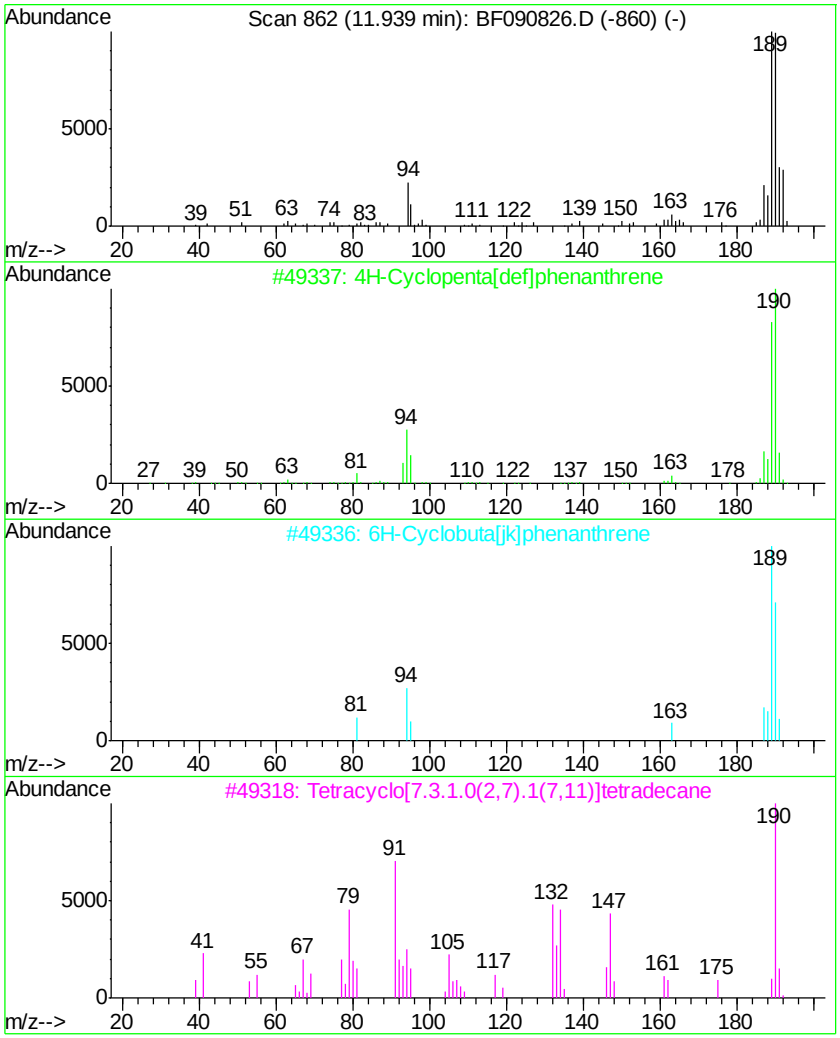
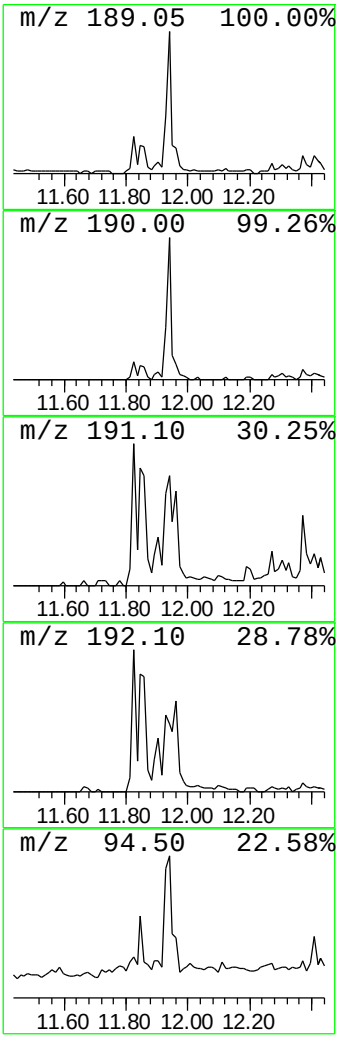
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.37 ng	162243	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Tetracyclo[7.3.1.0(2,7).1(7,11)]...	190	C14H22	041171-94-2	25
4	4,4'-Difluorobiphenyl	190	C12H8F2	000398-23-2	17
5	Hydrazinecarboxaldehyde, 2-[3-(m...	190	C4H6N4OS2	038362-25-3	14





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Sample : H5394-06
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Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

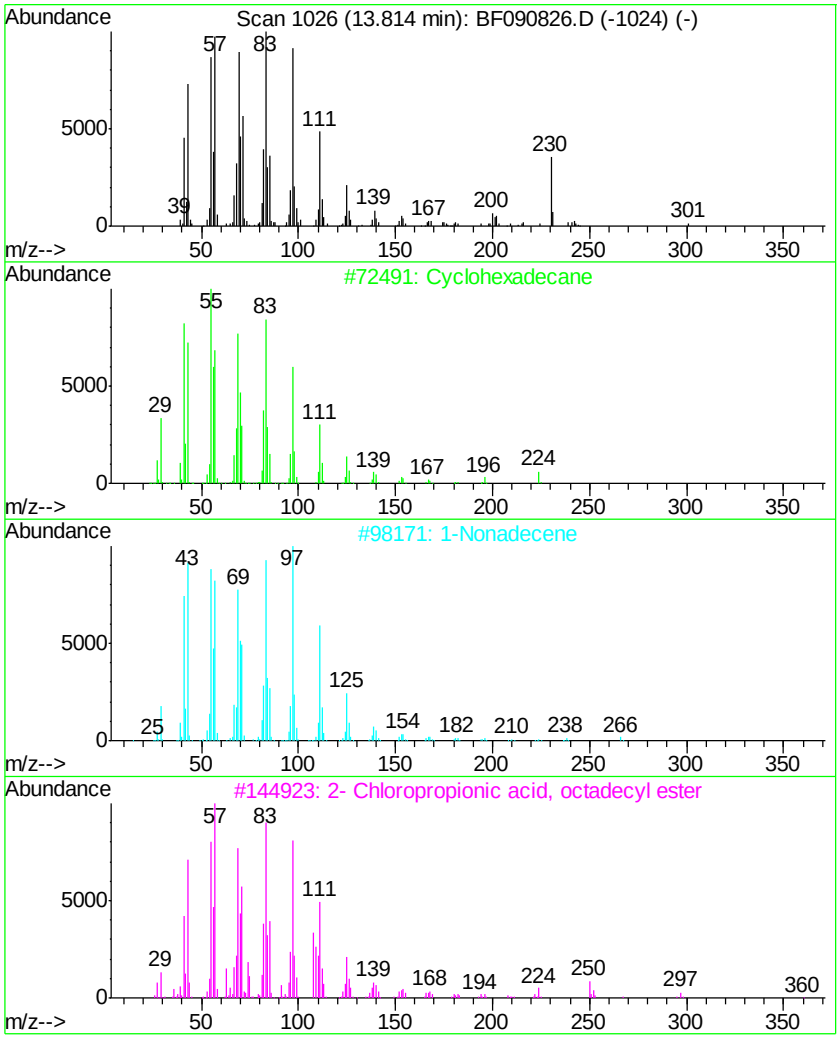
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

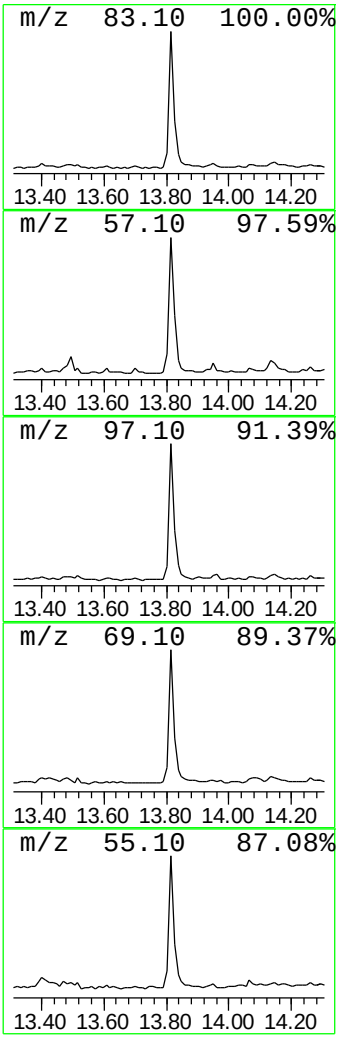
****

Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.09 ng	357113	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Nonadecene	266	C19H38	018435-45-5	93
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





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Data File : BF090826.D
Acq On : 25 Oct 2016 23:50
Operator : UM/SJ
Sample : H5394-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

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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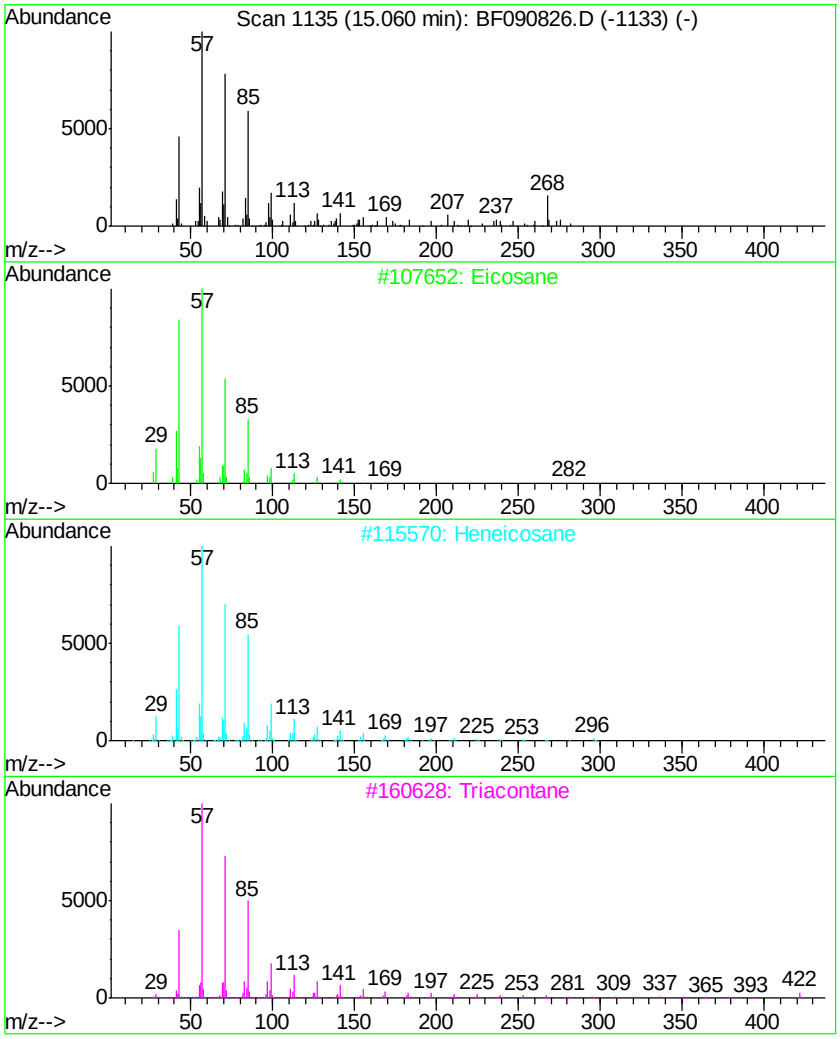
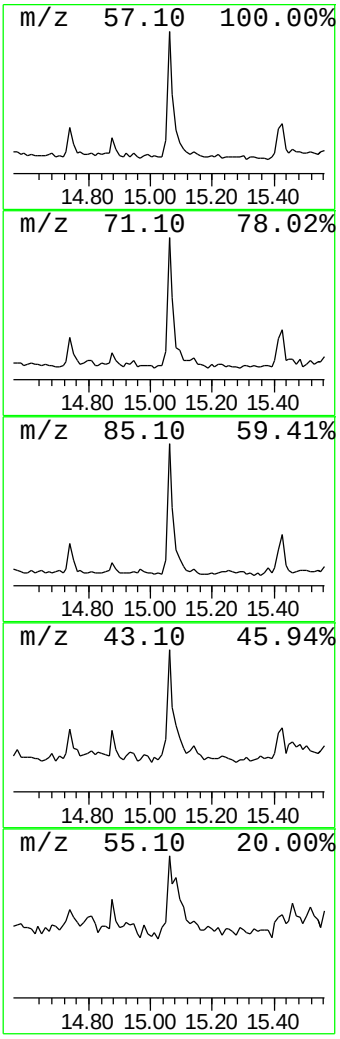
Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.58 ng	171562	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Nonacosane	408	C29H60	000630-03-5	87
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

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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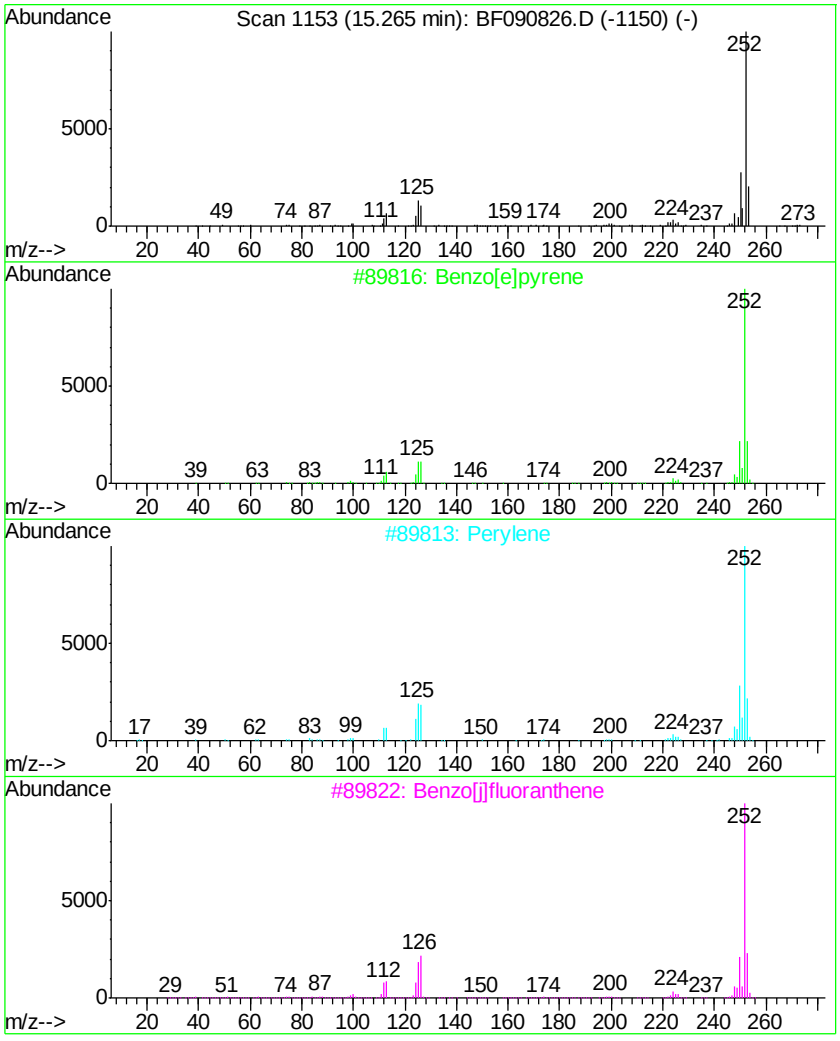
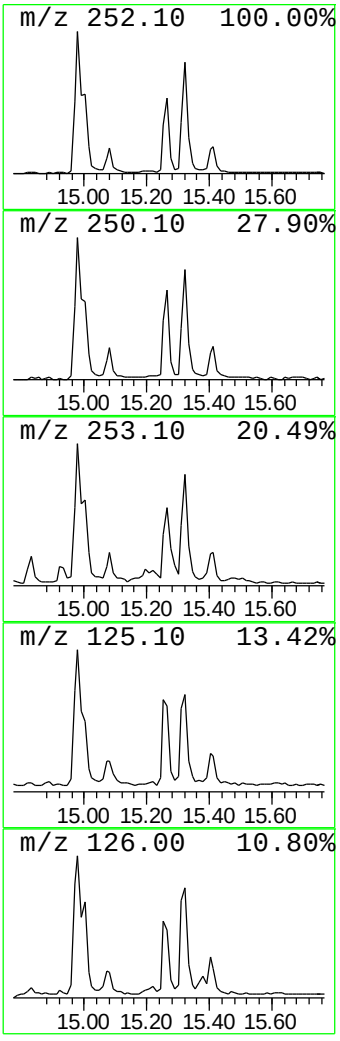
Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	4.07 ng	194985	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
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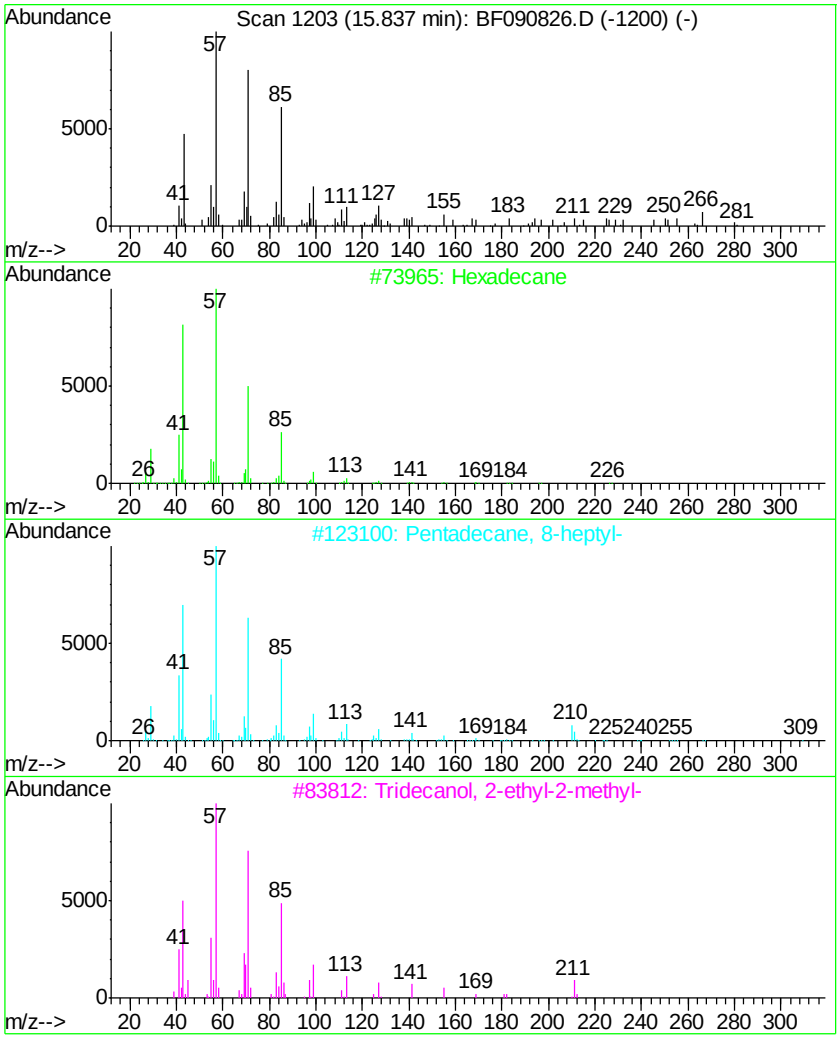
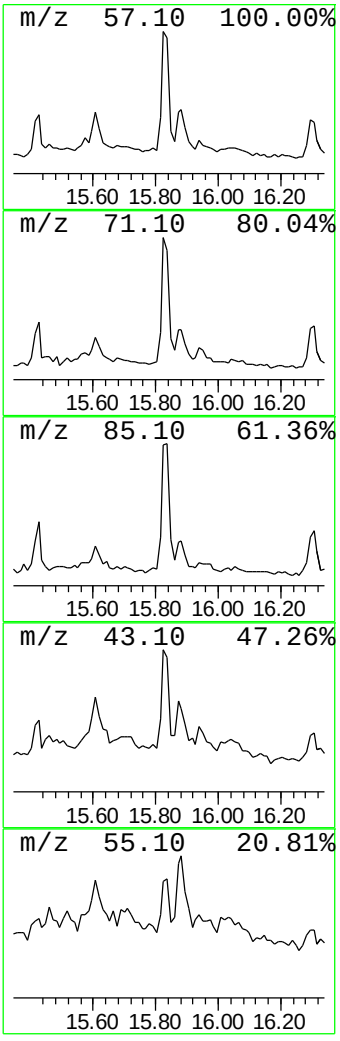
Peak Number 11 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.01 ng	96225	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Nonacosane	408	C29H60	000630-03-5	80





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Sample : H5394-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM-CENTER

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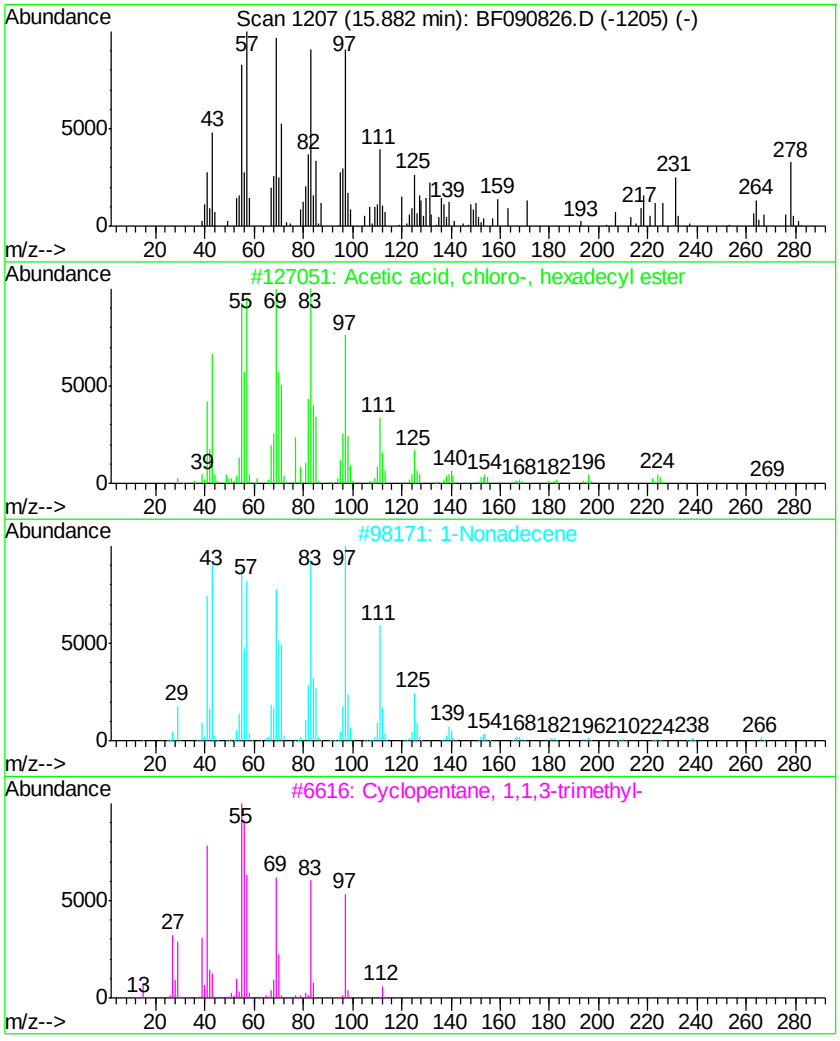
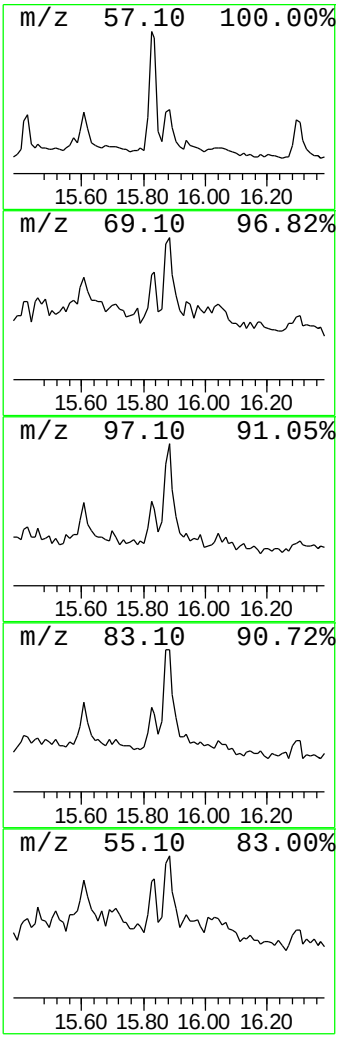
Peak Number 12 Acetic acid, chloro-, hexad... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.04 ng	97633	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	72
2	1-Nonadecene	266	C19H38	018435-45-5	58
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	53
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	52
5	1-Docosene	308	C22H44	001599-67-3	46





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Misc :
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ClientSampleId : BOTTOM-CENTER

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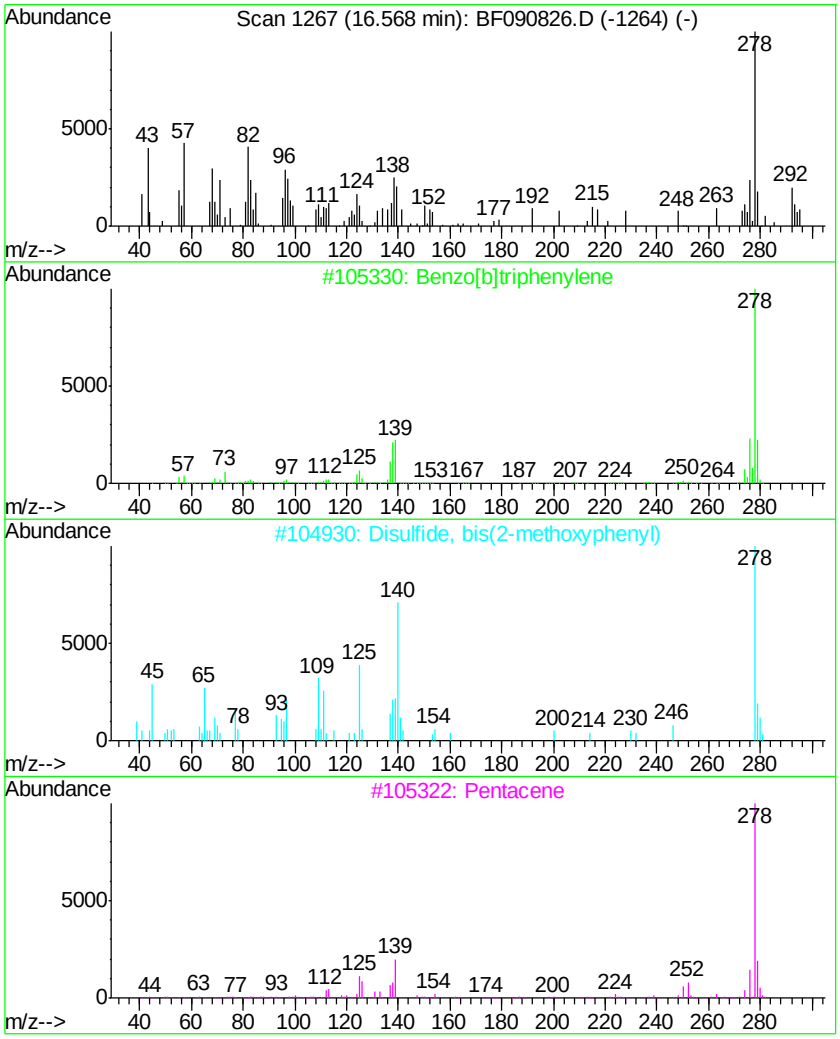
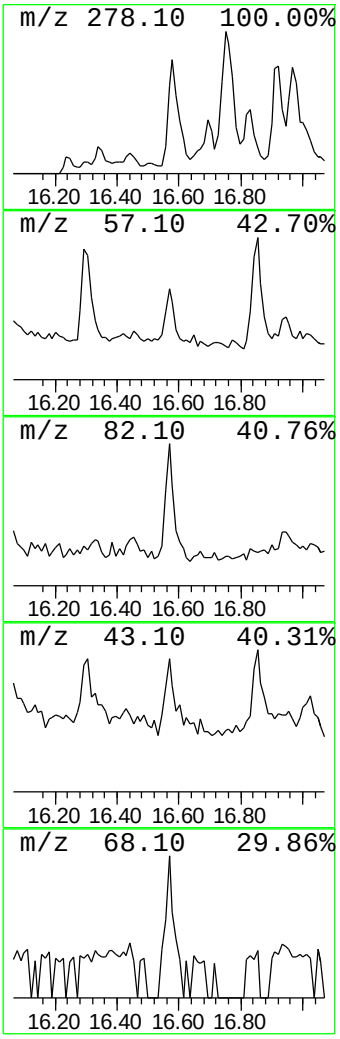
Peak Number 13 Benzo[b]triphenylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	2.25 ng	107797	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]triphenylene	278	C22H14	000215-58-7	53
2	Disulfide, bis(2-methoxyphenyl)	278	C14H14O2S2	013920-94-0	49
3	Pentacene	278	C22H14	000135-48-8	43
4	Dibenzo[b,h][1,6]naphthyridine, ...	278	C17H11ClN2	004240-91-9	43
5	2-(p-Methoxyphenyl)-4-quinolinec...	278	C17H14N2O2	051842-82-1	38





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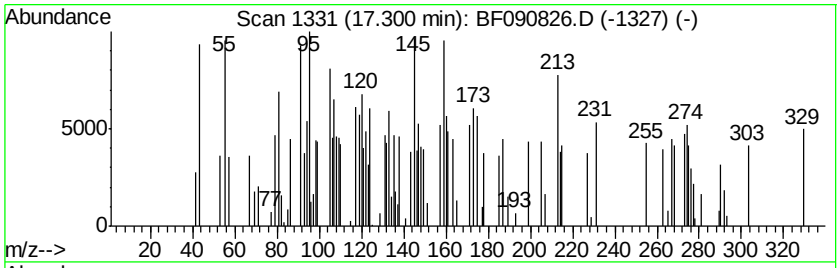
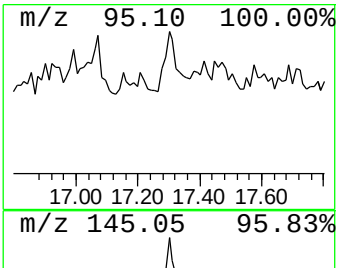
Peak Number 14 unknown17.30 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.21 ng	105657	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	35
2	2,4-Diamino-5-[3,4-methoxymethyl...	274	C13H14N4O3	071525-13-8	12
3	4-(4-Fluorophenyl)-3-morpholin-4...	318	C17H19FN2O3	151054-91-0	10
4	N-(4-Bromobenzylidene)-p-toluidine	273	C14H12BrN	039128-27-3	10
5	Propionic acid 1-methyl-4-phenyl...	287	C18H25NO2	1000297-46-2	10





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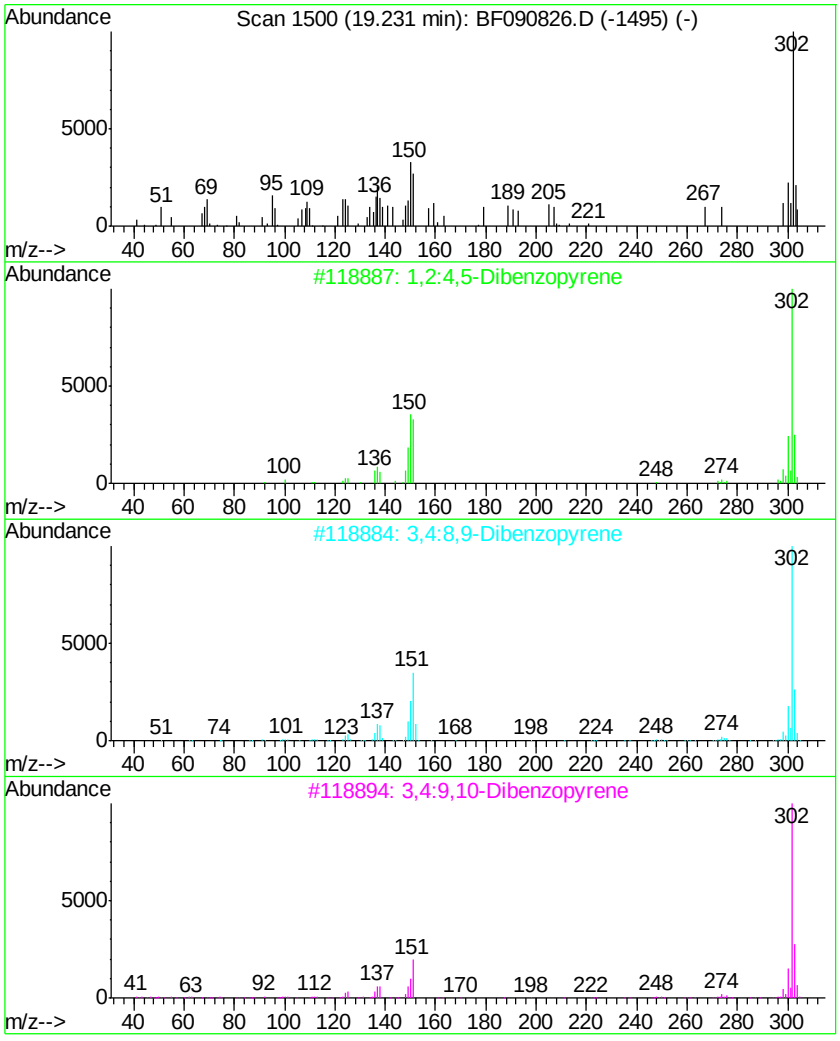
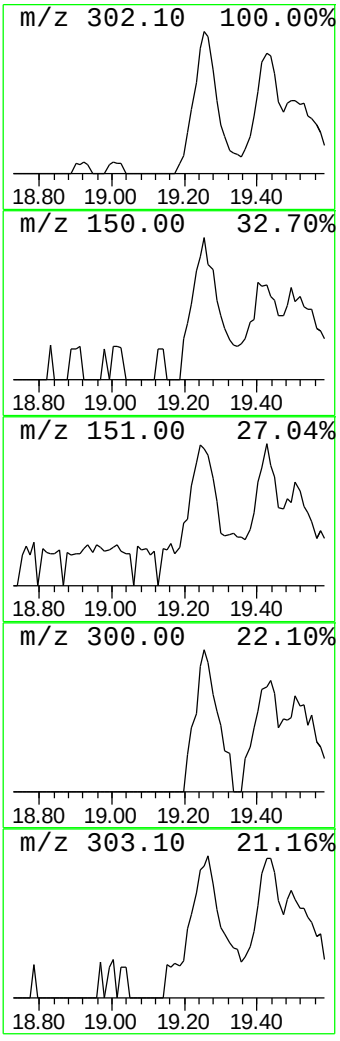
Peak Number 15 1,2:4,5-Dibenzopyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	2.89 ng	138441	Perylene-d12	15.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	89
2	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	64
3	3,4:9,10-Dibenzopyrene	302	C24H14	000189-55-9	58
4	1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	58
5	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	53





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	15.5	ng	738497	1	6.80	951246	20.0
unknown6.57	6.57	82.2	ng	3908340	1	6.80	951246	20.0
2,2,4-Trimethyl-1...	10.25	3.4	ng	255148	3	9.84	1498980	20.0
Dodecane, 2-methyl-	10.75	3.7	ng	252431	4	11.32	1367130	20.0
4H-Cyclopenta[def...	11.94	2.4	ng	162243	4	11.32	1367130	20.0
Cyclohexadecane	13.81	4.1	ng	357113	5	13.96	1744240	20.0
Eicosane	15.06	3.6	ng	171562	6	15.38	957759	20.0
Benzo[e]pyrene	15.27	4.1	ng	194985	6	15.38	957759	20.0
Hexadecane	15.84	2.0	ng	96225	6	15.38	957759	20.0
Acetic acid, chlo...	15.88	2.0	ng	97633	6	15.38	957759	20.0
Benzo[b]triphenylene	16.57	2.3	ng	107797	6	15.38	957759	20.0
unknown17.30	17.30	2.2	ng	105657	6	15.38	957759	20.0
1,2:4,5-Dibenzopy...	19.23	2.9	ng	138441	6	15.38	957759	20.0