LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101716\
Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

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-BF101316.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	5.091	238	241	251	rBV	813508	1048863	22.60%	1.388%
2	5.514	275	278	280	rBV	3821716	4191354	90.31%	5.547%
3	6.543	365	368	370	rBV	3757726	4214196	90.80%	5.577%
4	6.680	377	380	382	rBV	3274619	4267639	91.95%	5.648%
5	6.909	397	400	402	rBV	2379130	2170364	46.76%	2.872%
6	7.069	411	414	416	rBV	2029439	2819905	60.76%	3.732%
7	7.469	447	449	455	rBV	2189545	2354075	50.72%	3.115%
8	7.560	455	457	465	rVB2	56391	133096	2.87%	0.176%
9	8.200	510	513	515	rBV	2452857	3070675	66.16%	4.064%
10	8.474	535	537	541	rVB	100347	120241	2.59%	0.159%
11	8.909	573	575	579	rVB	83945	80257	1.73%	0.106%
12	9.012	582	584	586	rVB	55815	69713	1.50%	0.092%
13	9.275	604	607	609	rBV	3775221	3582800	77.20%	4.741%
14	9.389	615	617	619	rVB2	58993	63262	1.36%	0.084%
15	9.537	627	630	632	rBV	34787	56299	1.21%	0.075%
16	9.606	634	636	638	rVV	63299	84128	1.81%	0.111%
17	9.663	639	641	644	rVV	968534	922075	19.87%	1.220%
18	9.732	645	647	652	rVB3	28553	64916	1.40%	0.086%
19	9.812	652	654	657	rBV	131705	132486	2.85%	0.175%
20	9.880	657	660	663	rVB	72223	81568	1.76%	0.108%
21	9.949	664	666	668	rVV	2687133	3064415	66.03%	4.055%
22	9.983	668	669	671	rVB	295131	234745	5.06%	0.311%
23	10.155	682	684	686	rBV	126326	140905	3.04%	0.186%
24	10.360	700	702	703	rBV	56144	72141	1.55%	0.095%
25	10.383	703	704	705	rVB	136625	97438	2.10%	0.129%
26	10.498	712	714	717	rBV	192543	175091	3.77%	0.232%
27	10.600	721	723	727	rBV3	37307	81339	1.75%	0.108%
28	10.738	733	735	738	rBV	2046087	2167289	46.70%	2.868%
29	10.863	744	746	750	rVB	147258	254252	5.48%	0.336%
30	11.046	760	762	763	rBV	55818	67549	1.46%	0.089%
31	11.195	771	775	778	rBV4	27015	53200	1.15%	0.070%
32	11.309	781	785	786	rBV2	118887	151572	3.27%	0.201%
33	11.332	786	787	790	rVB	81785	97948	2.11%	0.130%
34	11.435	794	796	801	rBV2	1776061	3618088	77.96%	4.788%

LSC Area Percent Report

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Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

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 >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.515	802	803	805	rVB	307268	240730	5.19%	0.319%
36	11.663	814	816	821	rBV2	154041	245327	5.29%	0.325%
37	11.732	821	822	824	rVB	92149	75214	1.62%	0.100%
38	11.938	838	840	841	rBV	122671	119628	2.58%	0.158%
39	11.972	841	843	845	rVB	126662	146713	3.16%	0.194%
40	12.018	845	847	848	rBV2	63042	74399	1.60%	0.098%
41	12.052	848	850	854	rVB2	250474	376865	8.12%	0.499%
42	12.143	855	858	859	rBV	117100	140132	3.02%	0.185%
43	12.166	859	860	864	rVV3	62143	110353	2.38%	0.146%
44	12.441	881	884	885	rVB3	63078	95639	2.06%	0.127%
45	12.486	886	888	890	rBV	124764	170468	3.67%	0.226%
46	12.532	890	892	893	rBV	110822	122440	2.64%	0.162%
47	12.658	900	903	905	rBV	996354	1266012	27.28%	1.675%
48	12.692	905	906	909	rVB3	32751	63186	1.36%	0.084%
49	12.852	917	920	921	rBV	4630747	4370552	94.17%	5.784%
50	12.886	921	923	925	rVV	1042455	1562536	33.67%	2.068%
51	12.921	925	926	929	rVB2	710818	780849	16.82%	1.033%
52	13.024	933	935	939	rVV	2222413	2374126	51.15%	3.142%
53	13.104	939	942	946	rVB3	94435	209868	4.52%	0.278%
54	13.206	948	951	953	rBV2	220537	349006	7.52%	0.462%
55	13.264	953	956	959	rVV2	172245	373117	8.04%	0.494%
56	13.309	959	960	964	rVV2	135179	207415	4.47%	0.274%
57	13.401	967	968	970	rVB	62788	88226	1.90%	0.117%
58	13.561	980	982	984	rBV	2868581	3016343	64.99%	3.992%
59	13.606	984	986	987	rBV	362945	476891	10.28%	0.631%
60	13.721	994	996	1000	rBV2	100041	142056	3.06%	0.188%
61	13.824	1002	1005	1007	rBV3	218576	462624	9.97%	0.612%
62	13.926	1012	1014	1017	rVB	590958	710861	15.32%	0.941%
63	14.086	1024	1028	1034	rBV2	2891293	4641196	100.00%	6.142%
64	14.189	1035	1037	1038	rVV	170849	167214	3.60%	0.221%
65	14.246	1040	1042	1045	rVV	660607	620943	13.38%	0.822%
66	14.555	1067	1069	1071	rBV2	629388	643679	13.87%	0.852%
67	14.864	1094	1096	1097	rBV	536170	592866	12.77%	0.785%
68	15.127	1116	1119	1123	rBV	801848	1759984	37.92%	2.329%
69	15.195	1123	1125	1130	rVB2	546788	885772	19.08%	1.172%
70	15.424	1142	1145	1148	rVB	450161	709100	15.28%	0.938%
71	15.481	1148	1150	1153	rVV	626580	1026322	22.11%	1.358%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

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-BF101316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.549	1153	1156	1166	rVB2	1656619	3525179	75.95%	4.665%
73	16.007	1194	1196	1199	rBV	297830	441049	9.50%	0.584%
74	16.510	1238	1240	1243	rVB	190930	315174	6.79%	0.417%
75	16.681	1252	1255	1262	rVB2	164643	420517	9.06%	0.556%
76	16.990	1280	1282	1288	rVB2	196251	453481	9.77%	0.600%
77	17.172	1296	1298	1302	rBV	101337	182409	3.93%	0.241%
78	17.435	1318	1321	1329	rVB	151564	360603	7.77%	0.477%
79	17.573	1330	1333	1339	rVB2	256240	644790	13.89%	0.853%

Sum of corrected areas: 75565738

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101716\
Data File : BF090620.D
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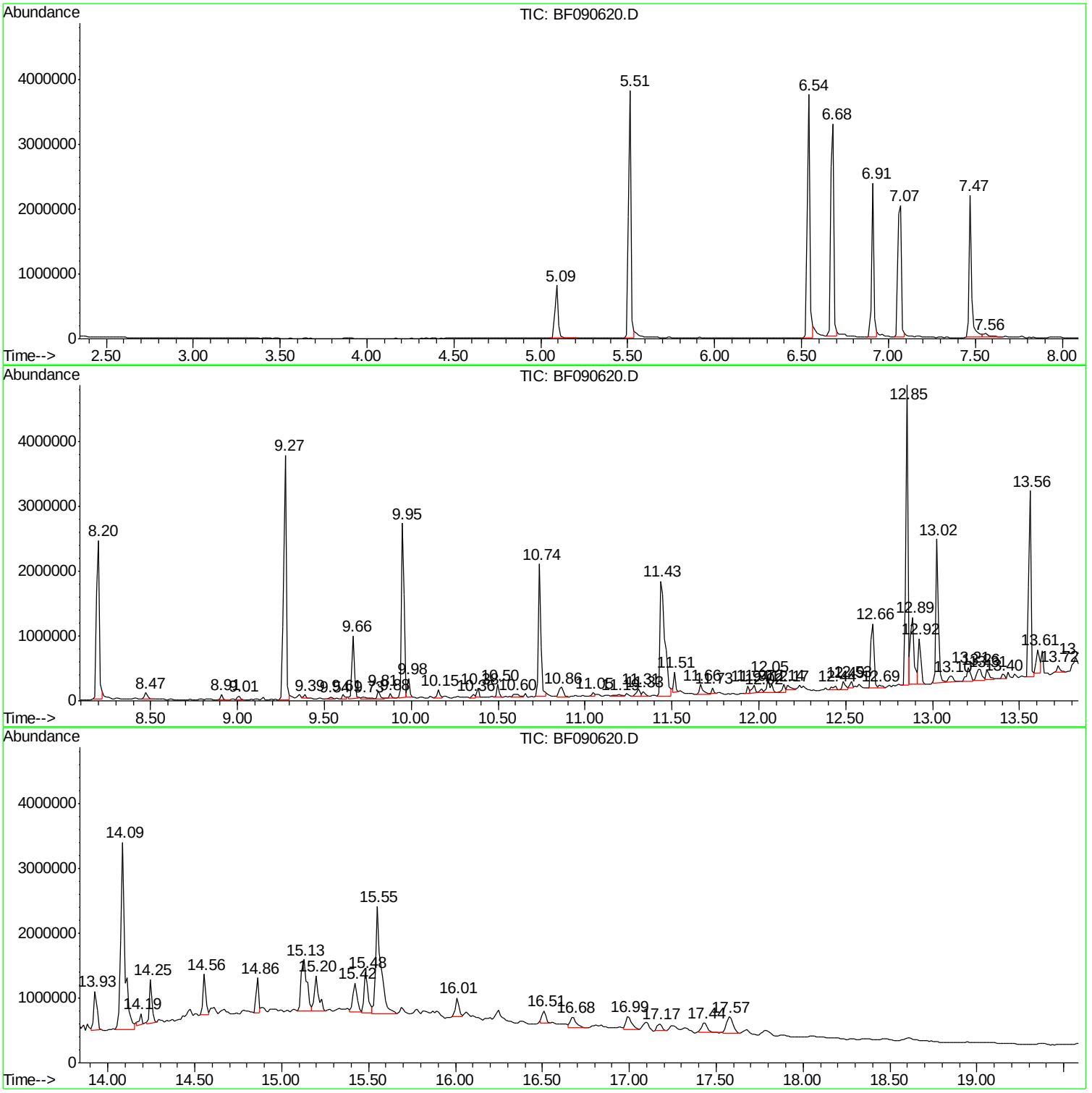
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101716\
Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

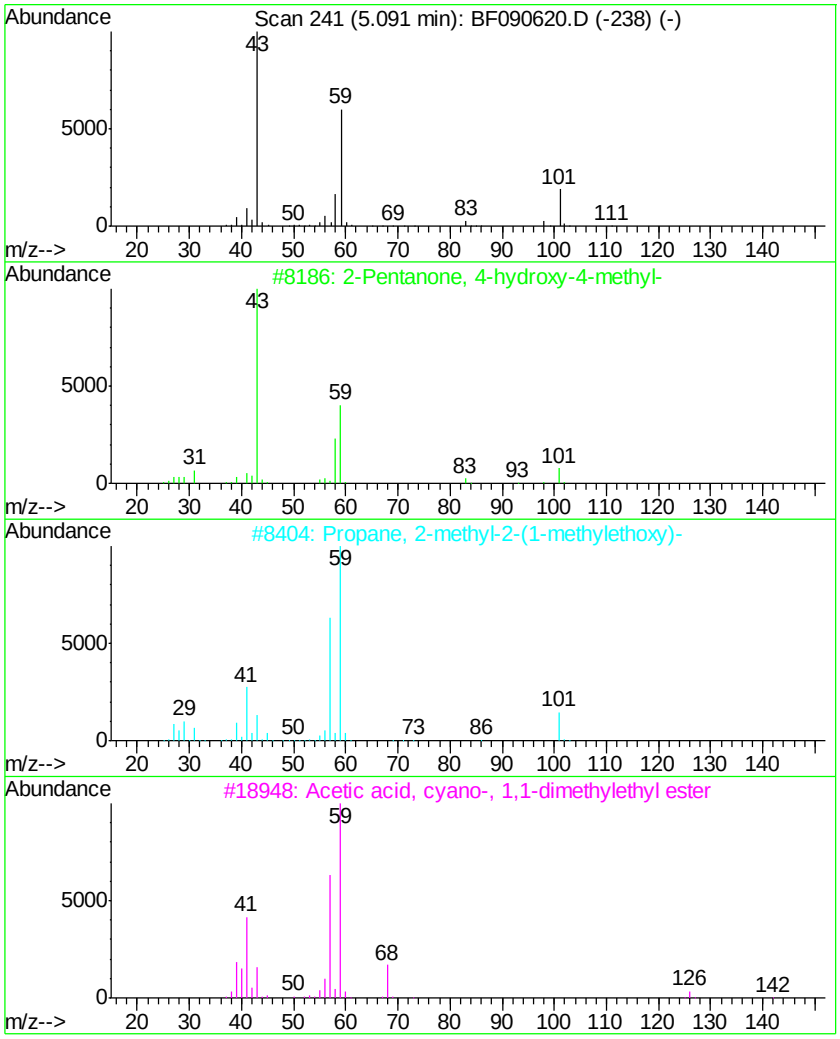
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

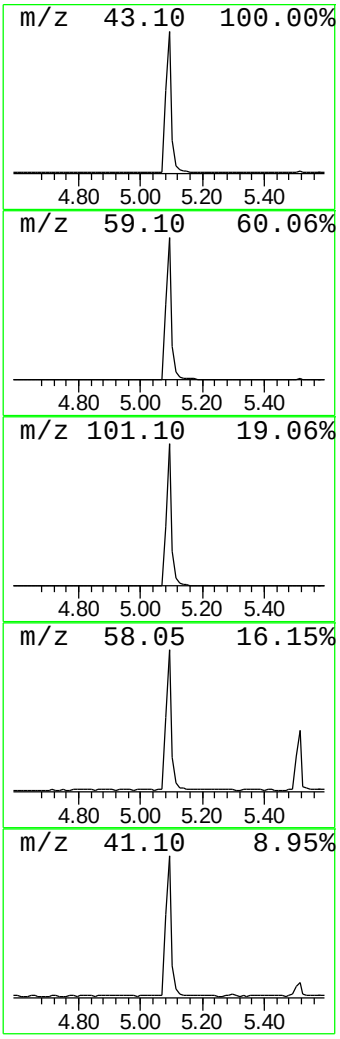
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	9.67 ng	1048860	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 17 Oct 2016 21:02
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Sample : H5227-01 2X
Misc :
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Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
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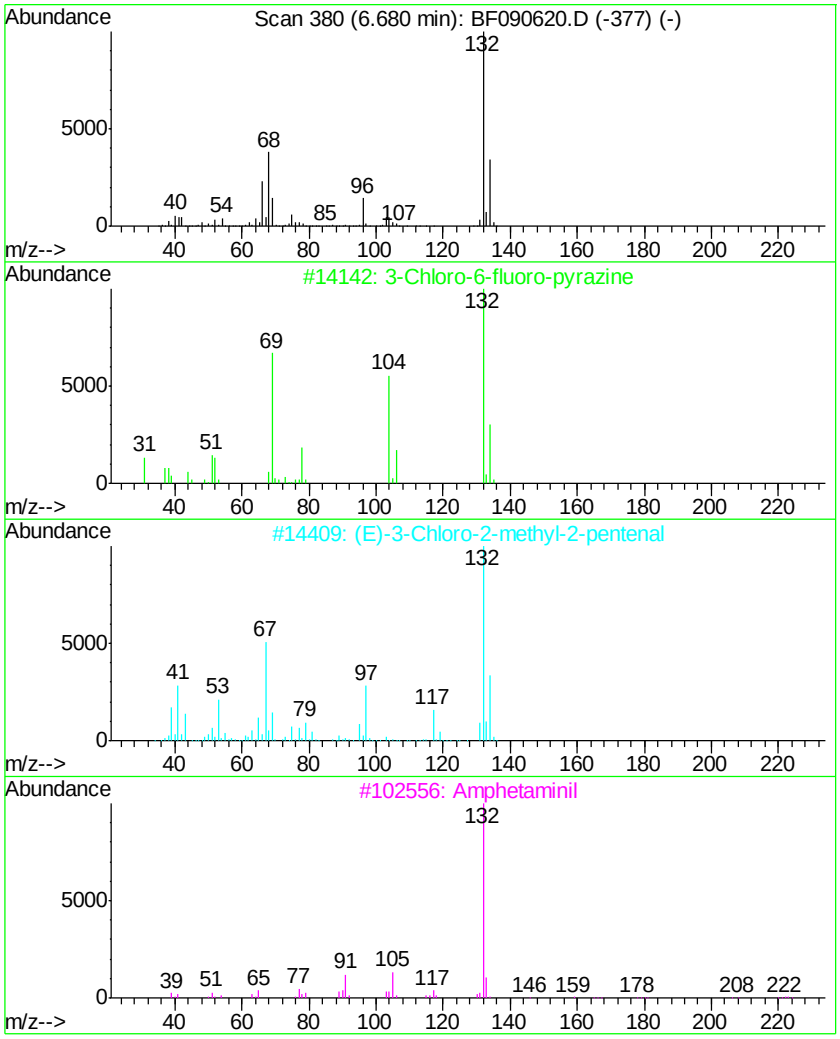
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

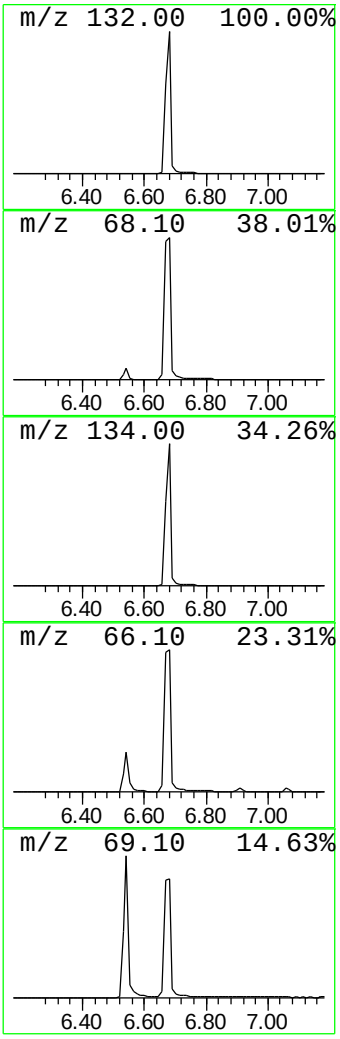
****

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	39.33 ng	4267640	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Acq On : 17 Oct 2016 21:02
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Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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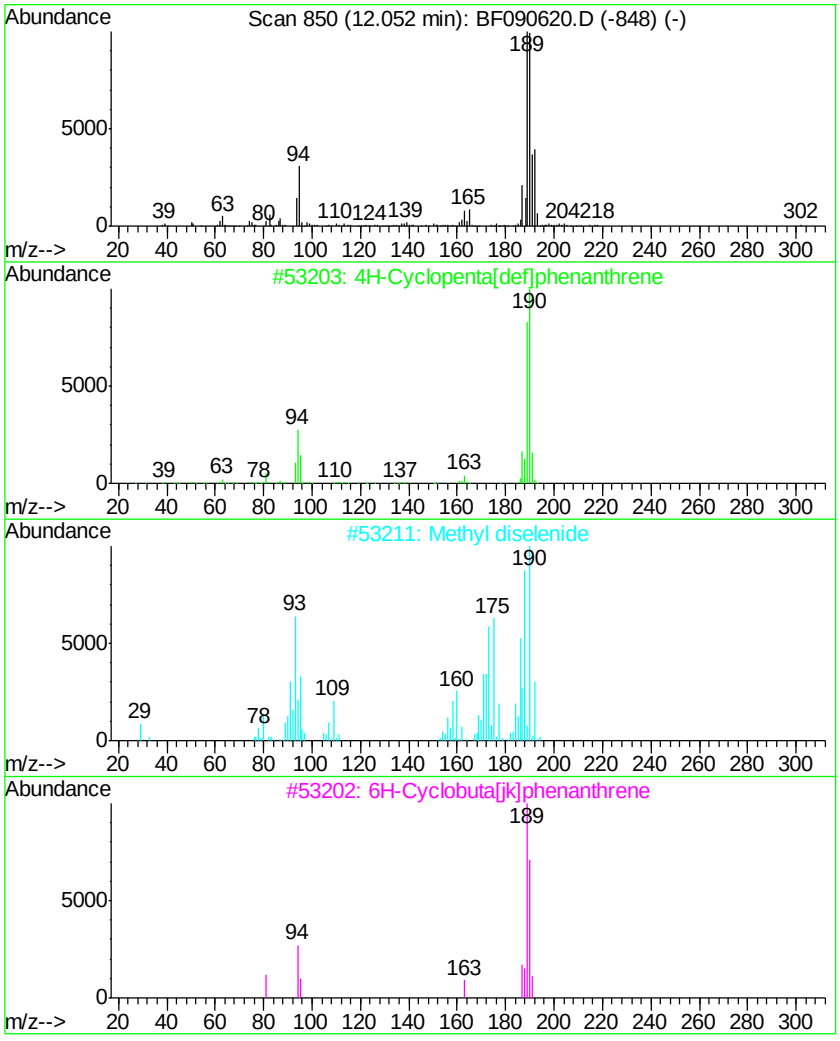
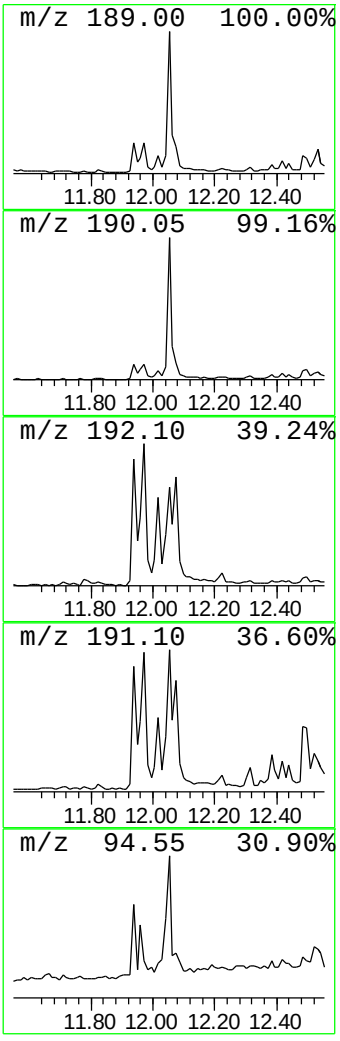
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.08 ng	376865	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Methyl diselenide	190	C2H6Se2	007101-31-7	46
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	17





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Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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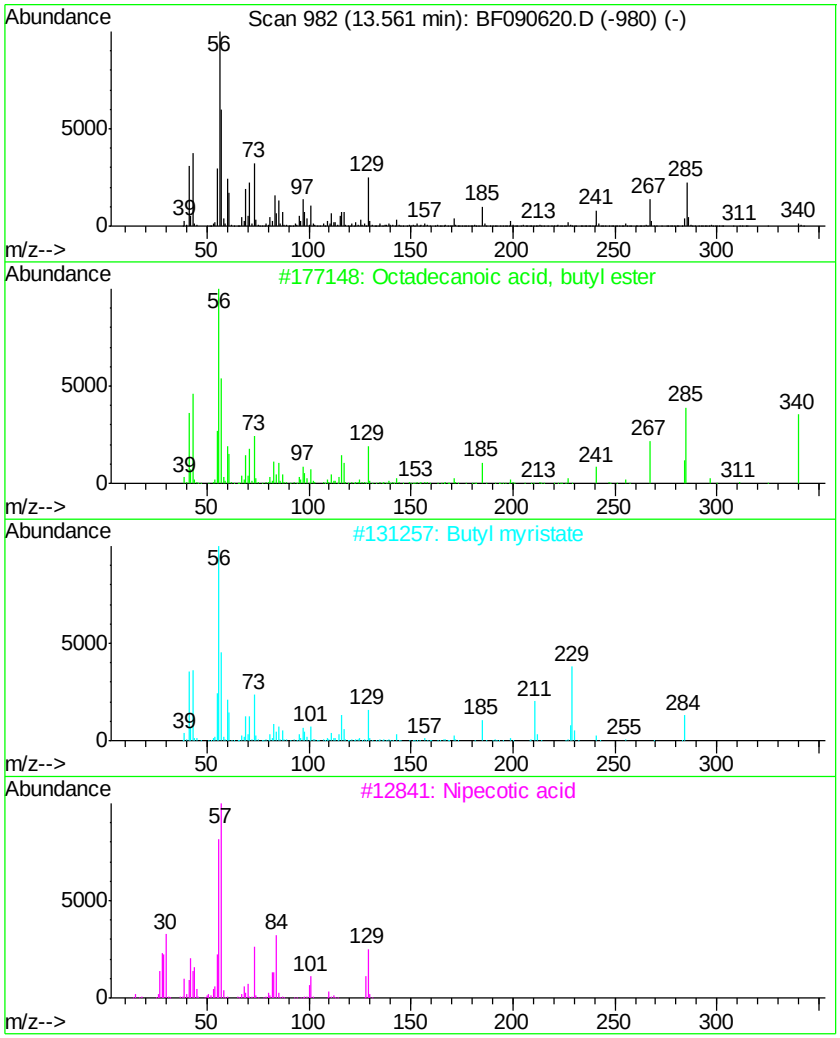
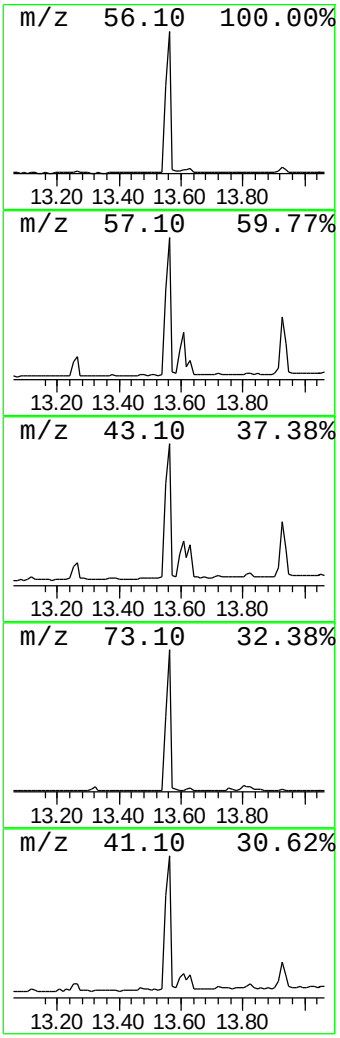
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	13.00 ng	3016340	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	50
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





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Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

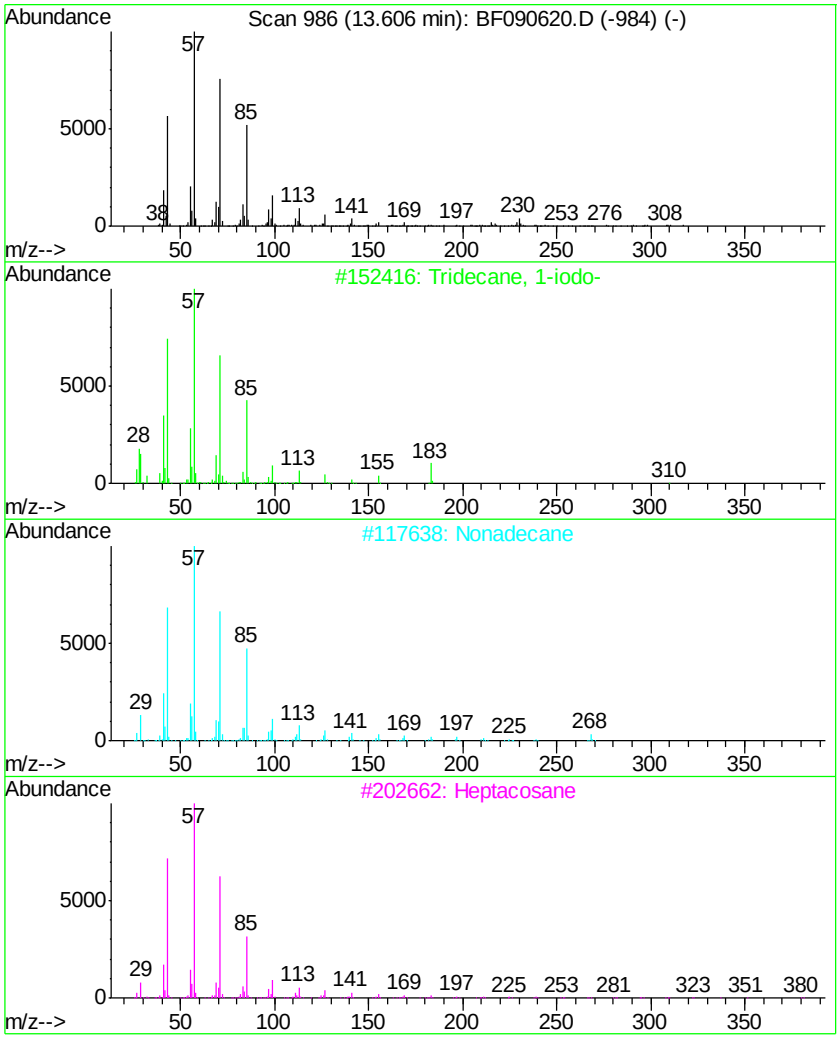
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

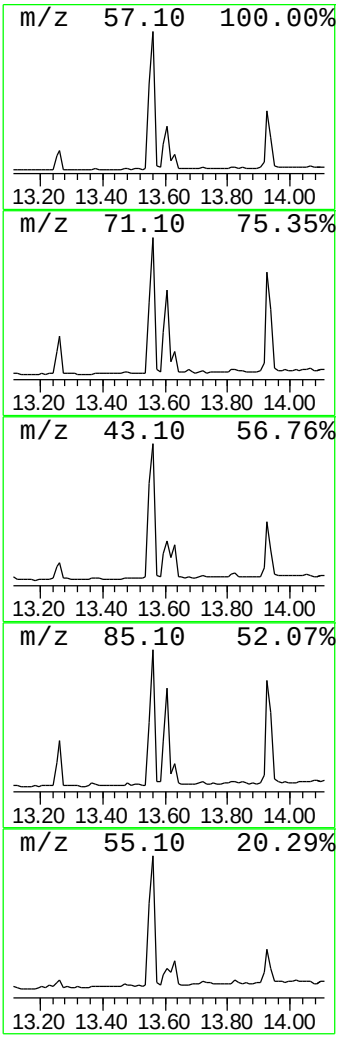
****

Peak Number 6 Tridecane, 1-iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.06 ng	476891	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2	Nonadecane	268	C19H40	000629-92-5	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101716\
Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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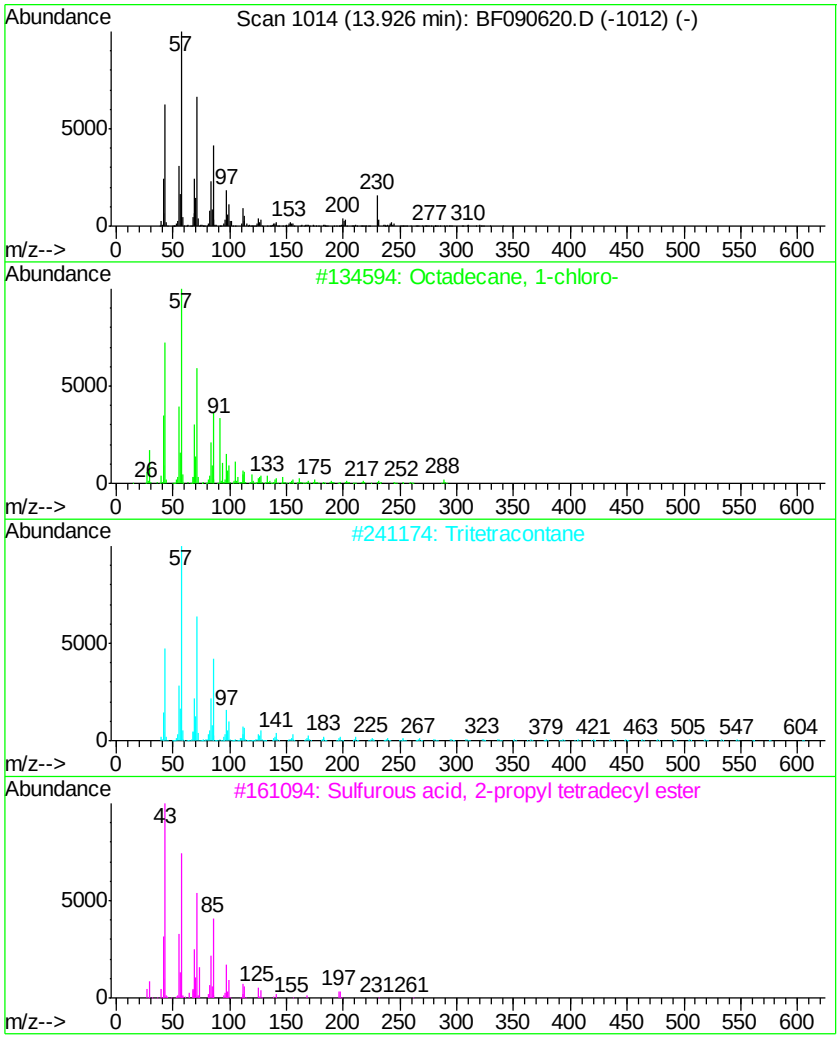
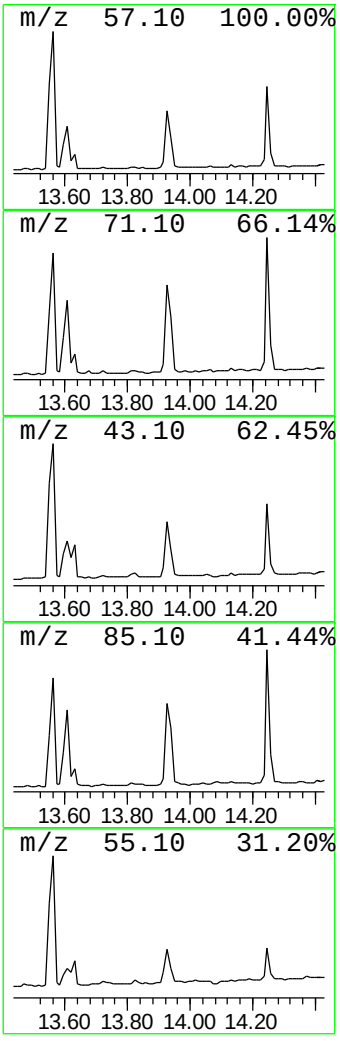
Peak Number 7 Octadecane, 1-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.06 ng	710861	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
2	Tritetracontane	605	C43H88	007098-21-7	86
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	70
5	Hexadecane	226	C16H34	000544-76-3	58





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Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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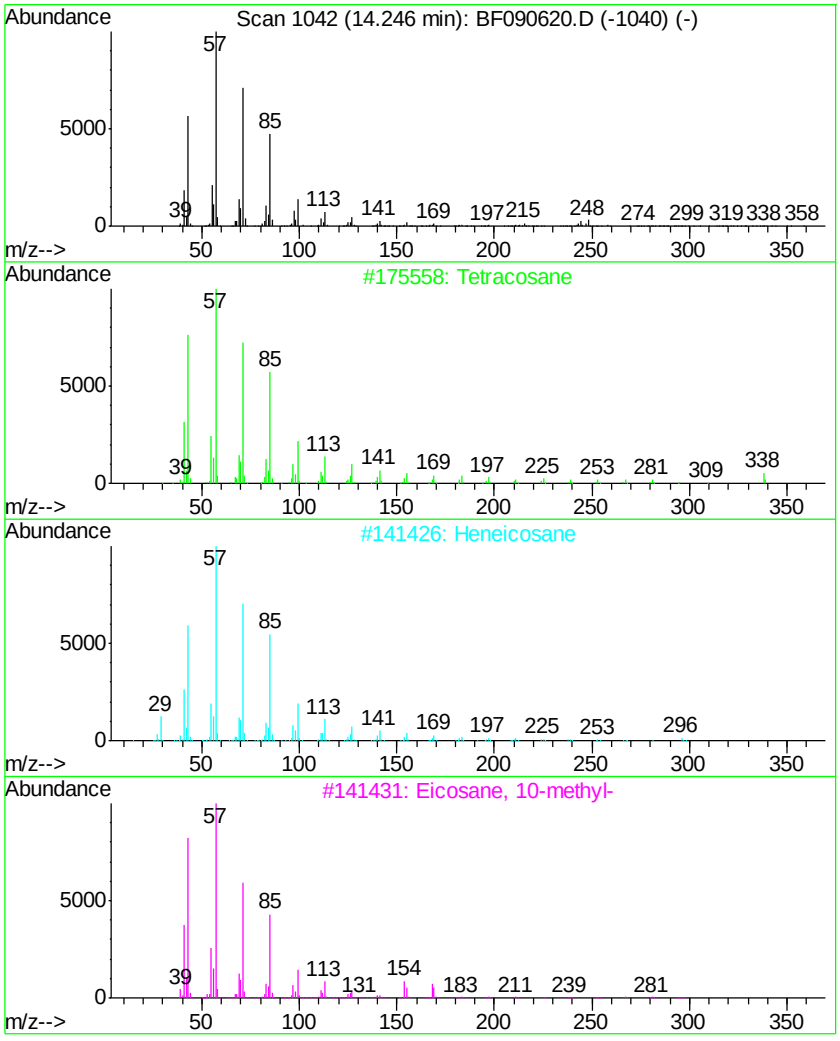
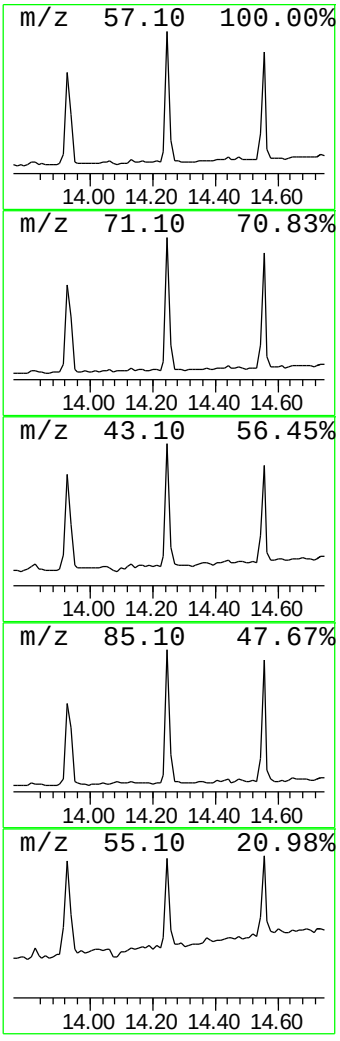
Peak Number 8 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.68 ng	620943	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Hexadecane	226	C16H34	000544-76-3	86





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Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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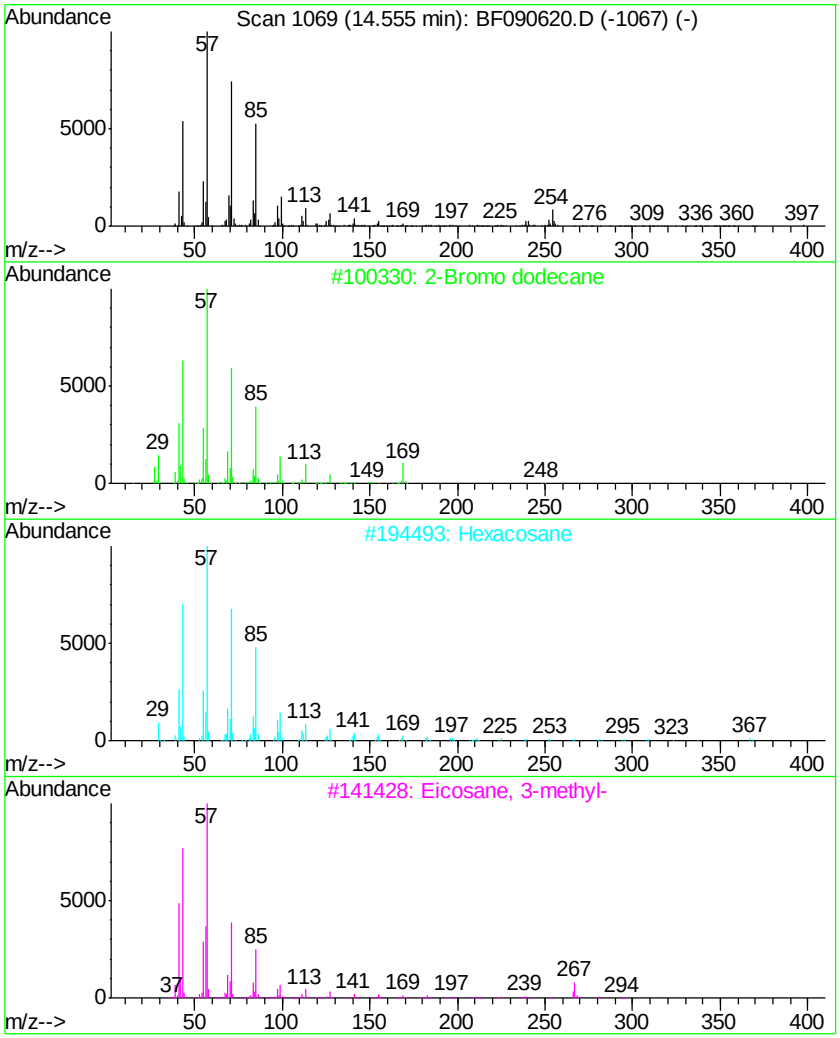
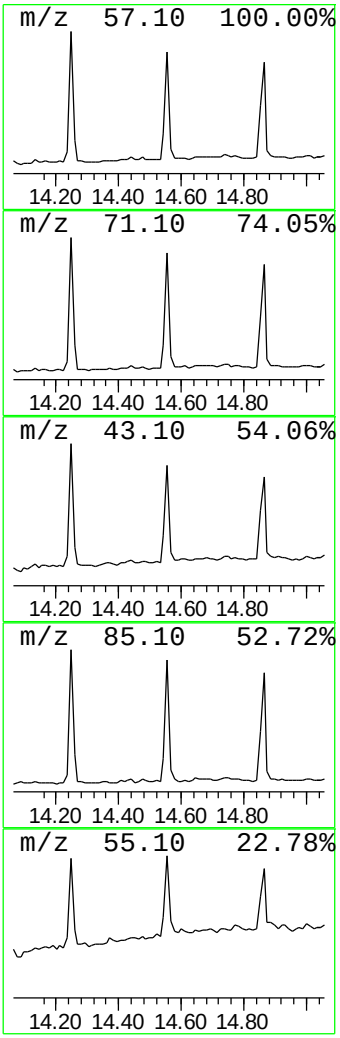
Peak Number 9 2-Bromo dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.77 ng	643679	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Eicosane, 3-methyl-	296	C21H44	006418-46-8	90
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90





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Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
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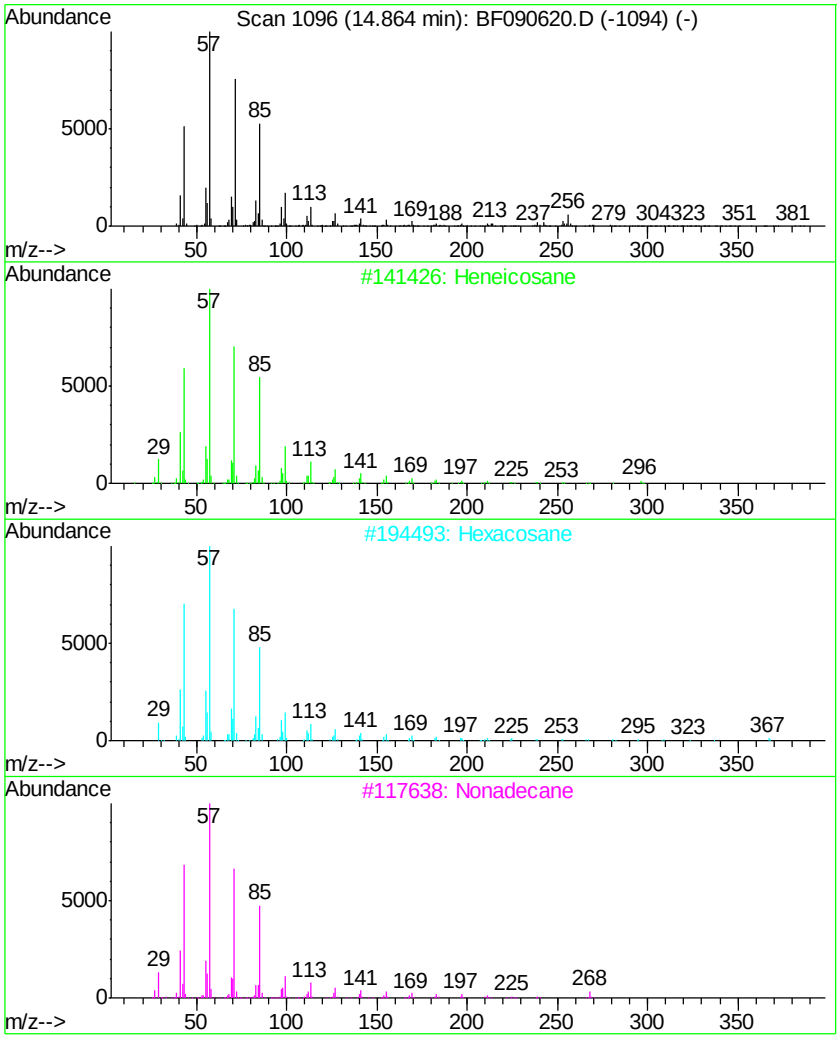
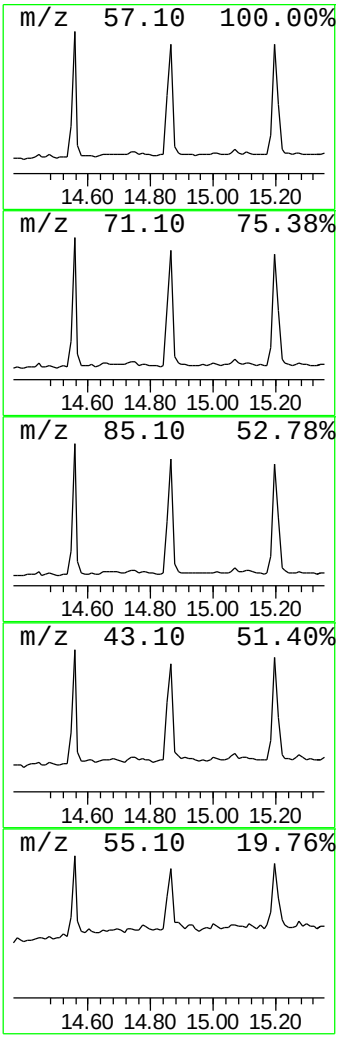
Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.36 ng	592866	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86





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Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
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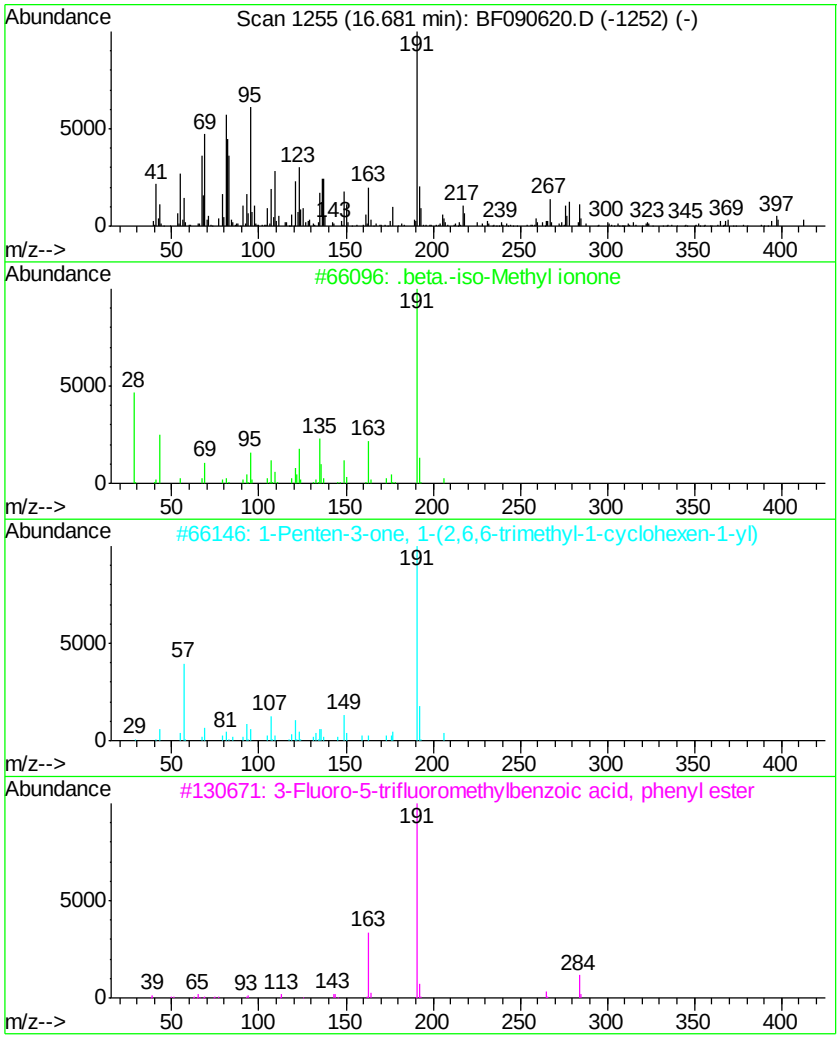
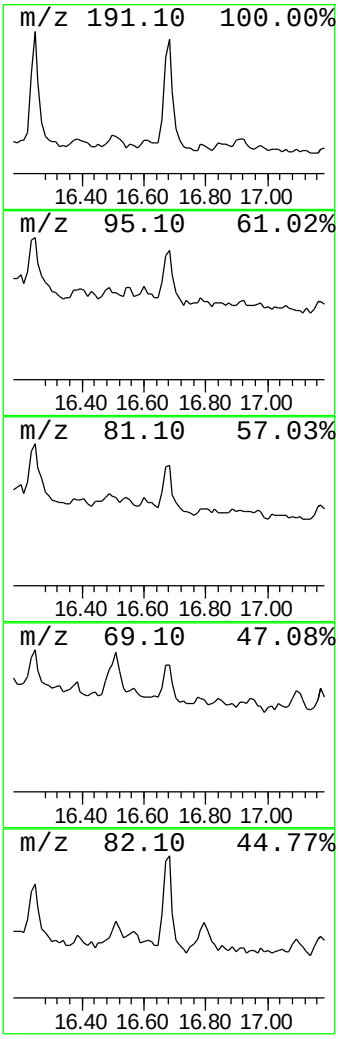
Peak Number 13 unknown16.68 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.68	2.39 ng	420517	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
3	3-Fluoro-5-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-95-5	35
4	2-Fluoro-6-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-69-4	35
5	3-Fluoro-4-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-93-7	35





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Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
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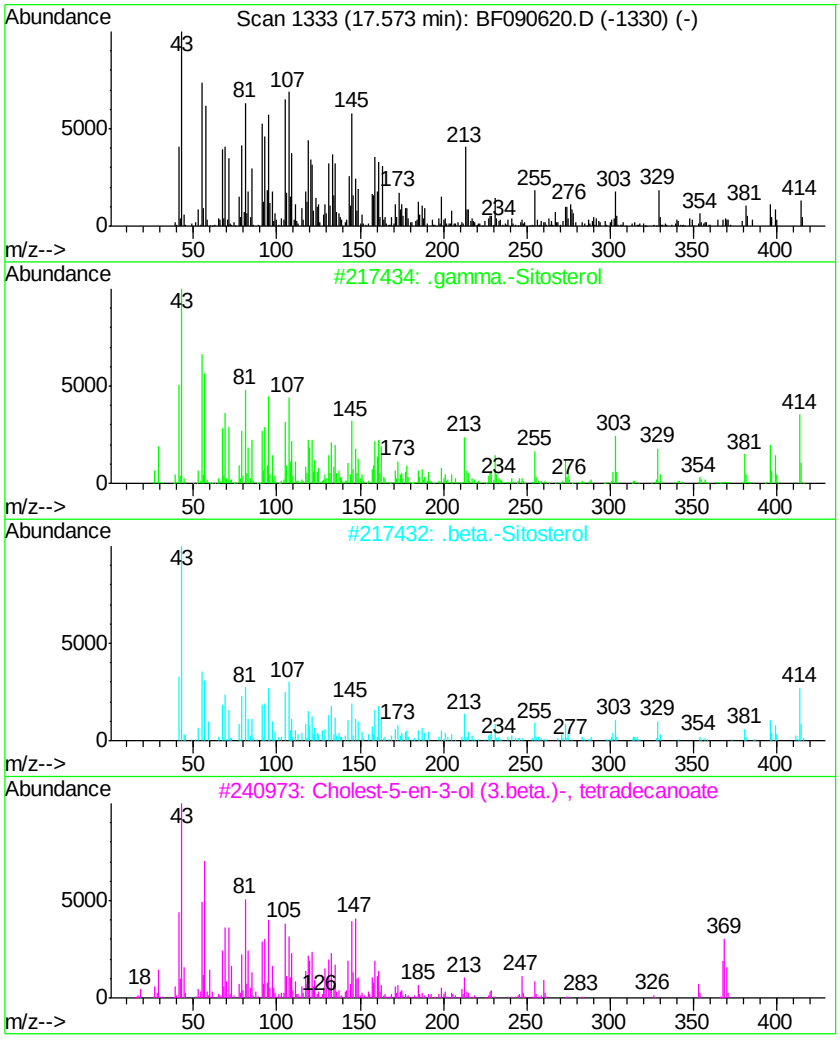
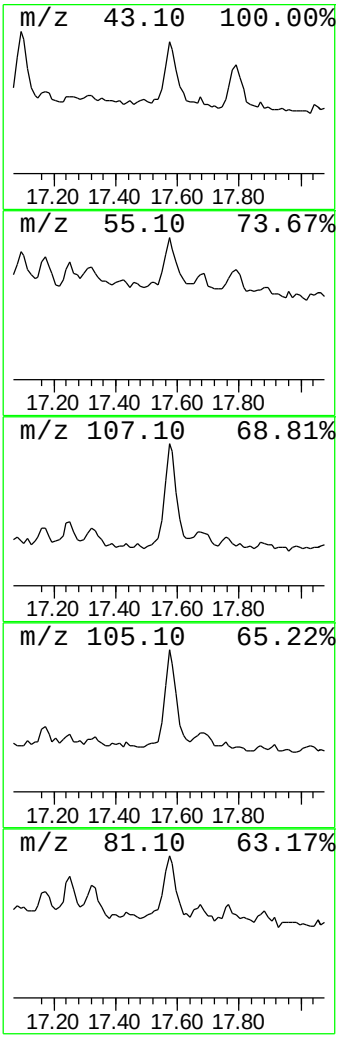
Peak Number 14 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	3.66 ng	644790	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	94
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	78
3	Cholest-5-en-3-ol (3.beta.)-, te...	597	C41H72O2	001989-52-2	53
4	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	52
5	Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	25





Tentatively Identified Compound (LSC) summary

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Data File : BF090620.D
Acq On : 17 Oct 2016 21:02
Operator : UM/SJ
Sample : H5227-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

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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
2-Pentanone, 4-hy...	5.09	9.7	ng	1048860	1	6.91	2170360	20.0
unknown6.68	6.68	39.3	ng	4267640	1	6.91	2170360	20.0
4H-Cyclopenta[def...	12.05	2.1	ng	376865	4	11.45	3618090	20.0
Octadecanoic acid...	13.56	13.0	ng	3016340	5	14.09	4641200	20.0
Tridecane, 1-iodo-	13.61	2.1	ng	476891	5	14.09	4641200	20.0
Octadecane, 1-chl...	13.93	3.1	ng	710861	5	14.09	4641200	20.0
Tetracosane	14.25	2.7	ng	620943	5	14.09	4641200	20.0
2-Bromo dodecane	14.56	2.8	ng	643679	5	14.09	4641200	20.0
Heneicosane	14.86	3.4	ng	592866	6	15.55	3525180	20.0
unknown16.68	16.68	2.4	ng	420517	6	15.55	3525180	20.0
.gamma.-Sitosterol	17.57	3.7	ng	644790	6	15.55	3525180	20.0