LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095284.D
Acq On : 20 May 2017 2:28
Operator : SJ/MA
Sample : I3189-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

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-BF050217.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	3.478	253	262	271	rBV	21836	62328	2.81%	0.294%
2	5.119	537	541	561	rBV2	118250	315662	14.24%	1.491%
3	5.731	641	645	675	rBV	810010	1913759	86.34%	9.040%
4	7.301	908	912	929	rBV	1070147	1856922	83.78%	8.771%
5	7.425	929	933	945	rVB	1431692	2216496	100.00%	10.470%
6	7.760	986	990	1008	rVB	444614	566225	25.55%	2.675%
7	7.995	1026	1030	1048	rBV	1267154	1644301	74.18%	7.767%
8	8.660	1139	1143	1162	rBV	671809	1108524	50.01%	5.236%
9	9.783	1329	1334	1353	rBV	413225	691006	31.18%	3.264%
10	11.548	1629	1634	1655	rBV	1476687	2129957	96.10%	10.061%
11	12.248	1749	1753	1768	rBV	218575	344582	15.55%	1.628%
12	12.613	1810	1815	1821	rBV2	466515	694327	31.33%	3.280%
13	12.666	1821	1824	1831	rVB	53618	75372	3.40%	0.356%
14	13.448	1953	1957	1961	rBV2	37434	44964	2.03%	0.212%
15	13.518	1964	1969	1977	rBV	35997	52690	2.38%	0.249%
16	13.807	2011	2018	2022	rBV4	14259	26410	1.19%	0.125%
17	13.907	2031	2035	2055	rBV	599775	1032366	46.58%	4.877%
18	14.218	2084	2088	2091	rBV	37790	48528	2.19%	0.229%
19	14.948	2208	2212	2217	rBV	36395	43161	1.95%	0.204%
20	15.012	2217	2223	2227	rVV	439562	606341	27.36%	2.864%
21	15.054	2227	2230	2241	rVV	365575	528641	23.85%	2.497%
22	15.142	2241	2245	2256	rVB	85682	138657	6.26%	0.655%
23	15.448	2293	2297	2304	rVB2	21162	36206	1.63%	0.171%
24	15.607	2320	2324	2328	rBV	25146	28083	1.27%	0.133%
25	15.807	2354	2358	2361	rBV	18549	22993	1.04%	0.109%
26	15.848	2361	2365	2371	rVB	26664	37061	1.67%	0.175%
27	15.971	2383	2386	2395	rVB4	56849	105386	4.75%	0.498%
28	16.242	2429	2432	2441	rVB	16864	24944	1.13%	0.118%
29	16.748	2514	2518	2522	rVB	23225	25134	1.13%	0.119%
30	16.795	2522	2526	2537	rVB	372849	469446	21.18%	2.218%
31	17.101	2573	2578	2584	rBV	334887	432275	19.50%	2.042%
32	17.248	2600	2603	2607	rVB2	24275	23197	1.05%	0.110%
33	17.295	2607	2611	2613	rBV	21227	25211	1.14%	0.119%
34	17.330	2613	2617	2626	rVV	1158491	1314491	59.30%	6.209%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3189-06
Misc :
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Instrument : BNA_F
ClientSampleId : TP-13-14

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.565	2653	2657	2663	rVB	48078	62496	2.82%	0.295%
36	17.648	2666	2671	2676	rBV	40757	53214	2.40%	0.251%
37	17.718	2676	2683	2685	rBV3	42346	71282	3.22%	0.337%
38	18.230	2762	2770	2771	rBV6	15772	32690	1.47%	0.154%
39	18.395	2796	2798	2802	rVV2	26278	33214	1.50%	0.157%
40	18.430	2802	2804	2808	rVV	20800	33292	1.50%	0.157%
41	18.471	2808	2811	2816	rVB3	29871	42188	1.90%	0.199%
42	18.577	2825	2829	2838	rBV6	48039	105950	4.78%	0.500%
43	18.689	2842	2848	2851	rBV2	460055	709567	32.01%	3.352%
44	18.724	2851	2854	2865	rVB2	126983	241151	10.88%	1.139%
45	18.818	2866	2870	2875	rBV3	44346	65194	2.94%	0.308%
46	18.983	2894	2898	2902	rVB4	46256	61190	2.76%	0.289%
47	19.959	3061	3064	3071	rBV	103103	199754	9.01%	0.944%
48	20.312	3121	3124	3129	rBV	69496	76095	3.43%	0.359%
49	20.365	3129	3133	3141	rVB	287183	388455	17.53%	1.835%
50	20.824	3208	3211	3217	rVB3	76476	101075	4.56%	0.477%
51	20.953	3230	3233	3240	rVB2	105409	162859	7.35%	0.769%
52	23.841	3719	3724	3725	rBV4	28399	44740	2.02%	0.211%

Sum of corrected areas: 21170052

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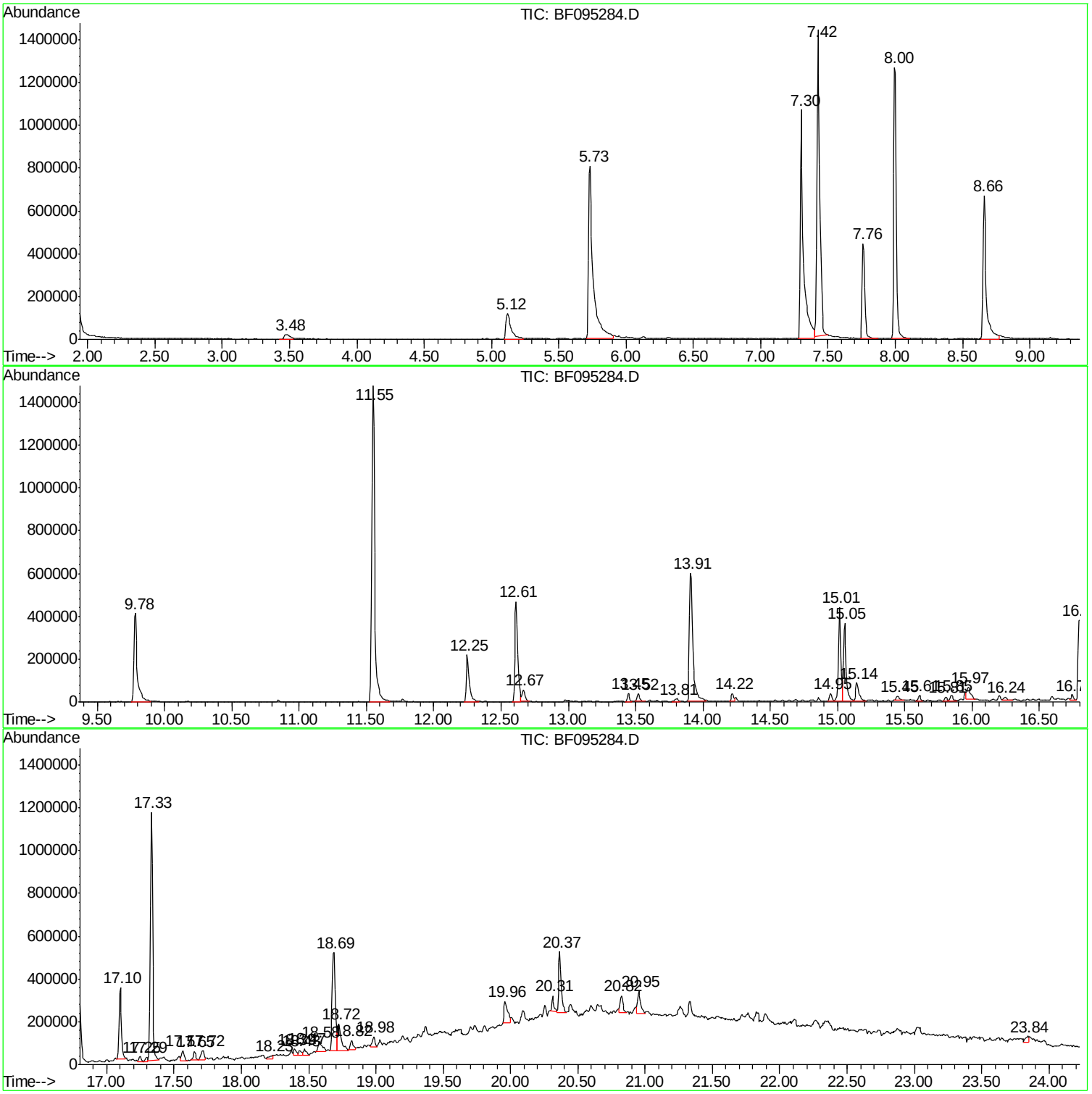
BNA_F
ClientSampleId :
TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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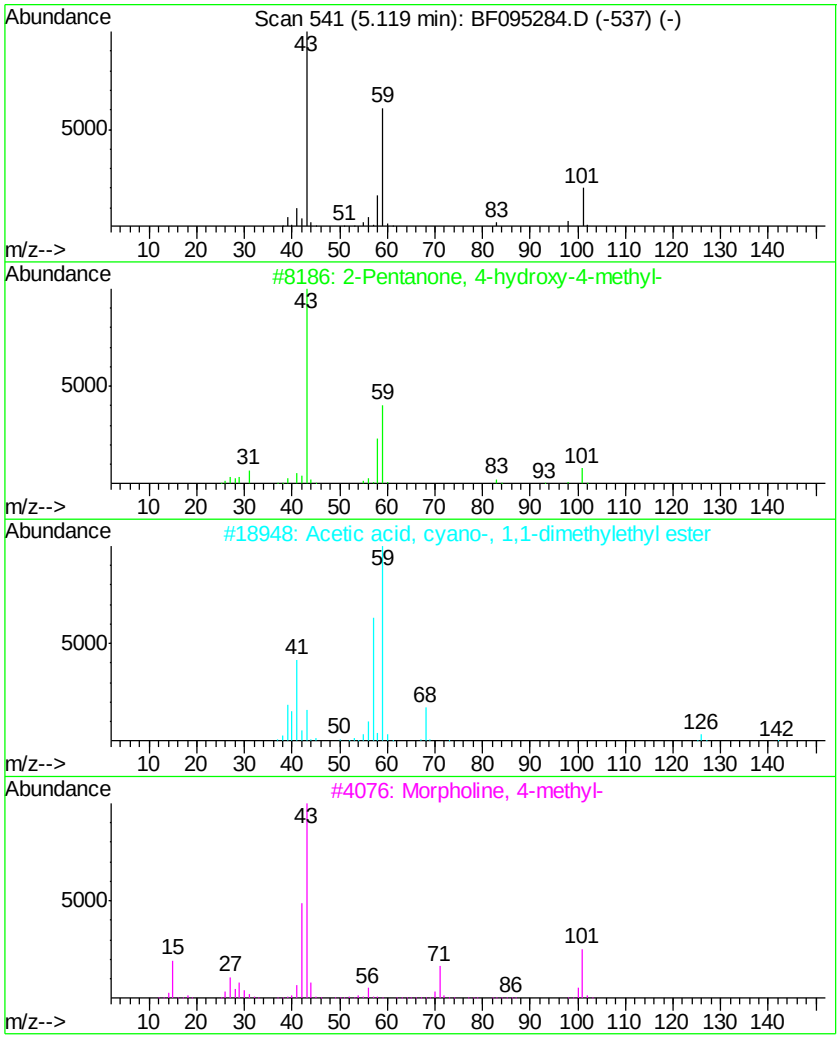
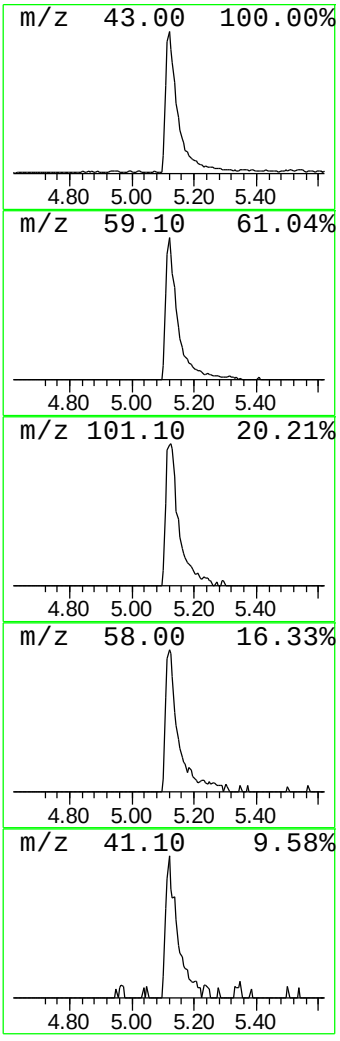
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	11.15 ng	315662	1,4-Dichlorobenzene-d4	7.76

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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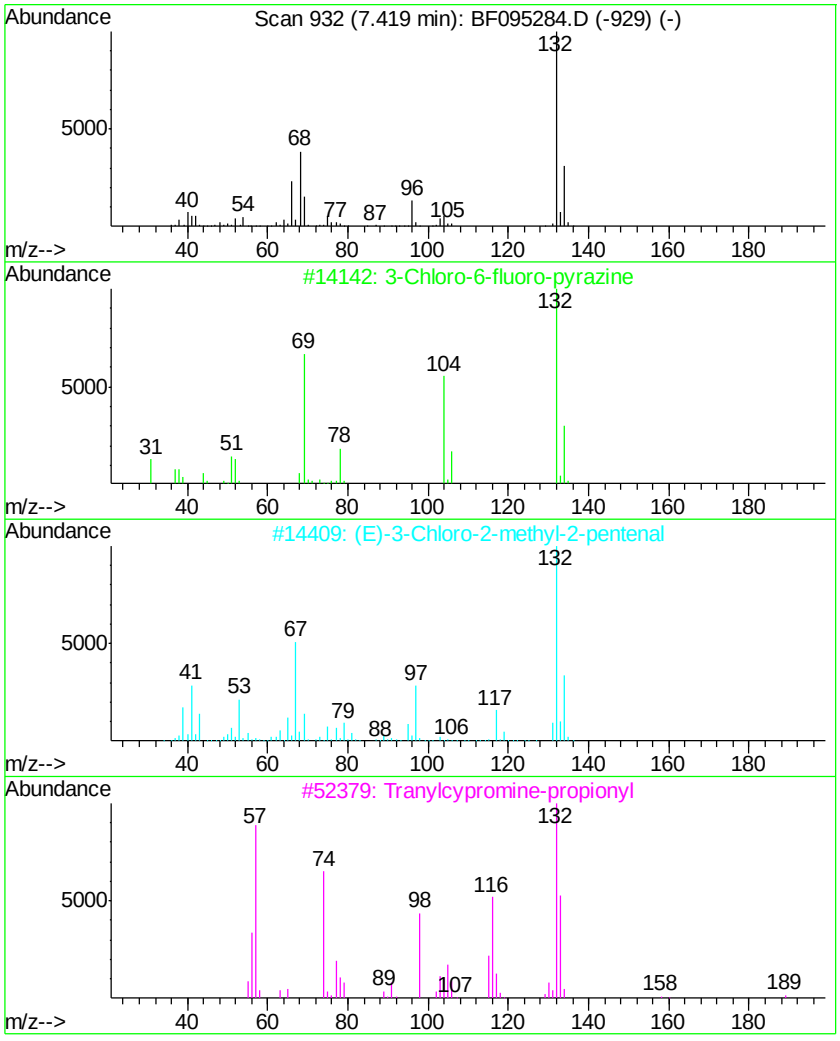
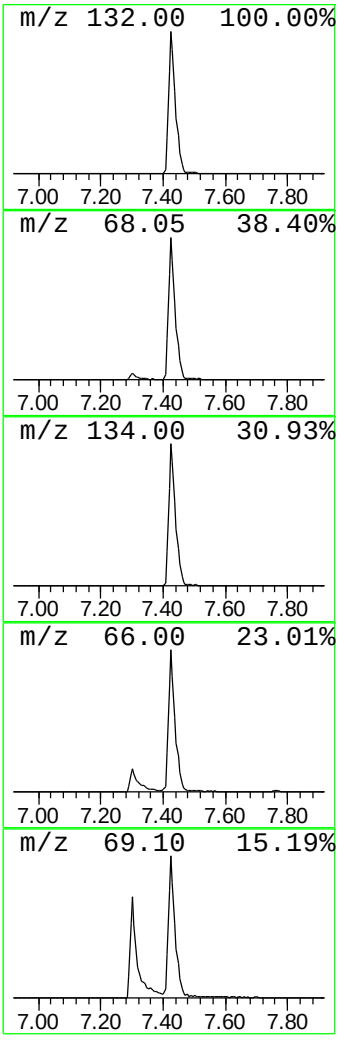
Peak Number 3 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	78.29 ng	2216500	1,4-Dichlorobenzene-d4	7.76

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : I3189-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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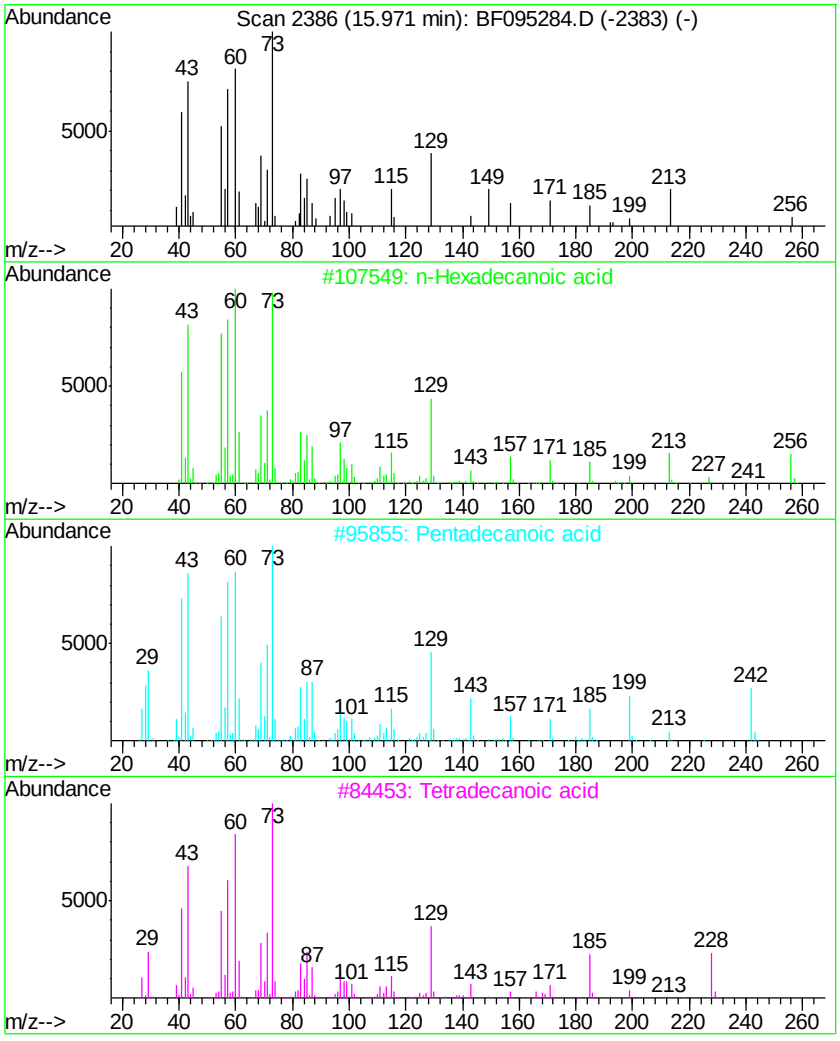
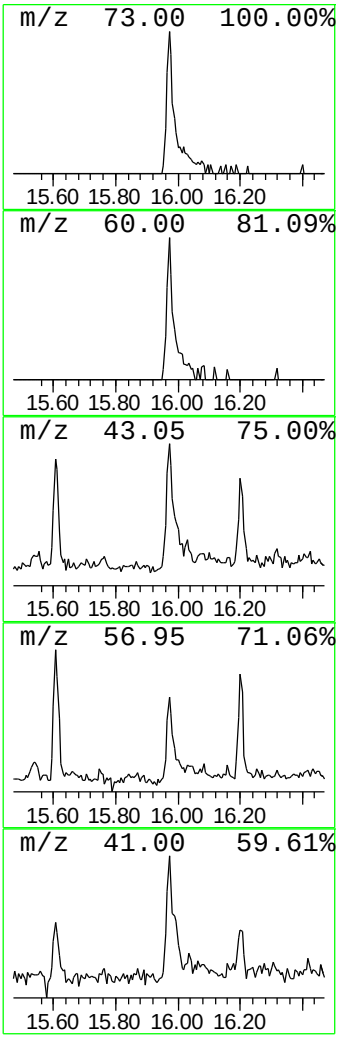
Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.48 ng	105386	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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Sample : I3189-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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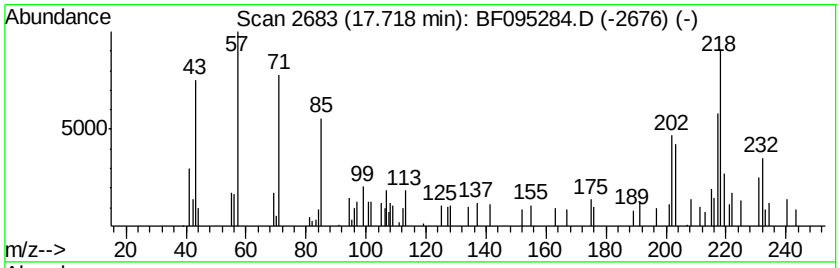
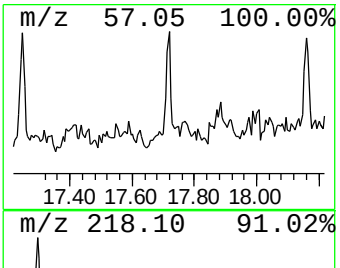
Peak Number 7 9-Phenyl-5H-benzocycloheptene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	2.01 ng	71282	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	55
2	7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	55
3	1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	55
4	Heptadecane	240	C17H36	000629-78-7	38
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	18





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Sample : I3189-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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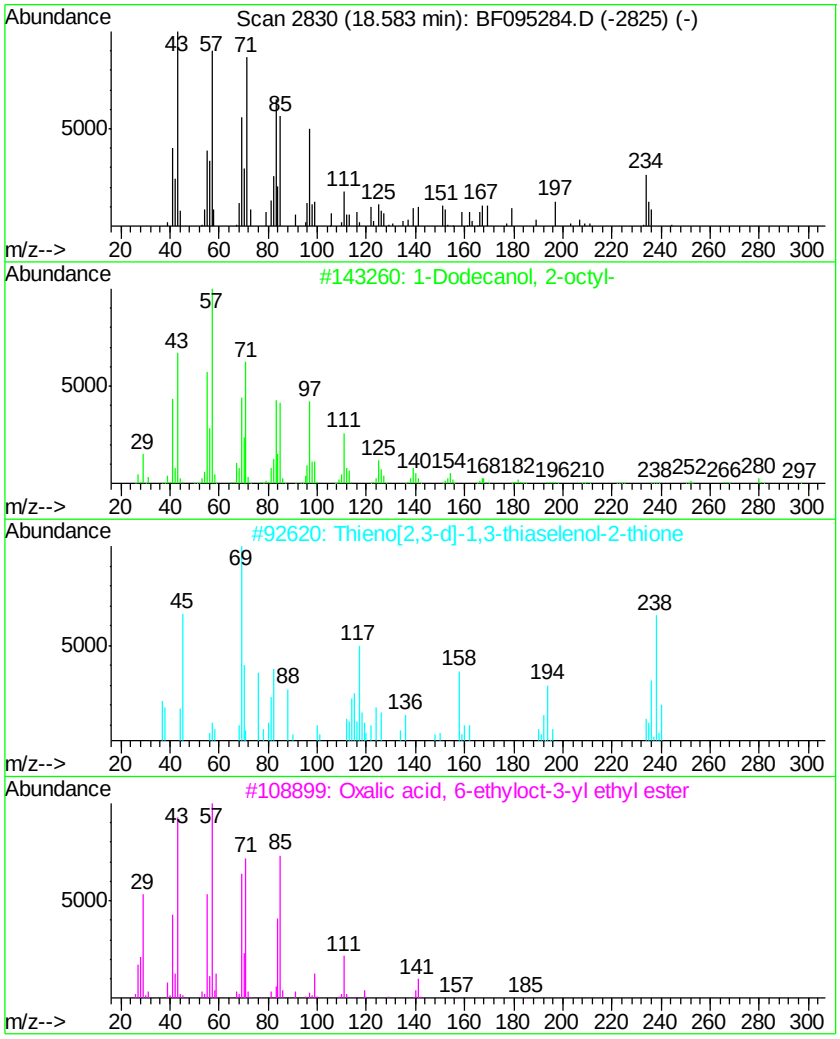
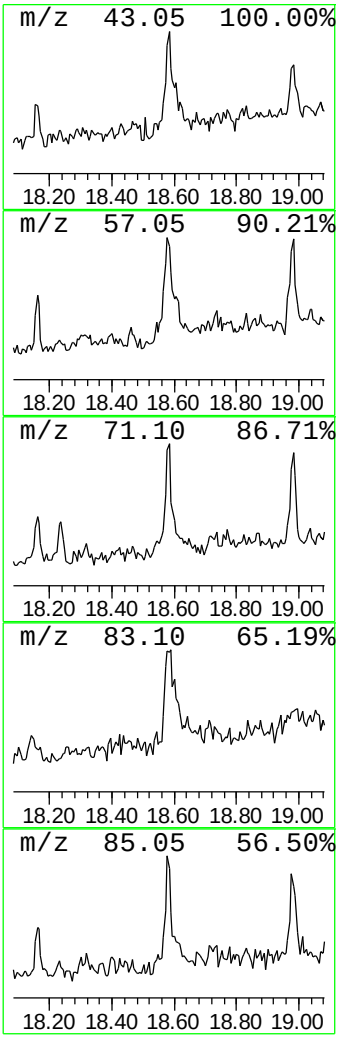
Peak Number 8 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.99 ng	105950	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	58
2	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
3	Oxalic acid, 6-ethyloct-3-yl eth...	258	C14H26O4	1000309-33-9	52
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	47
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	46





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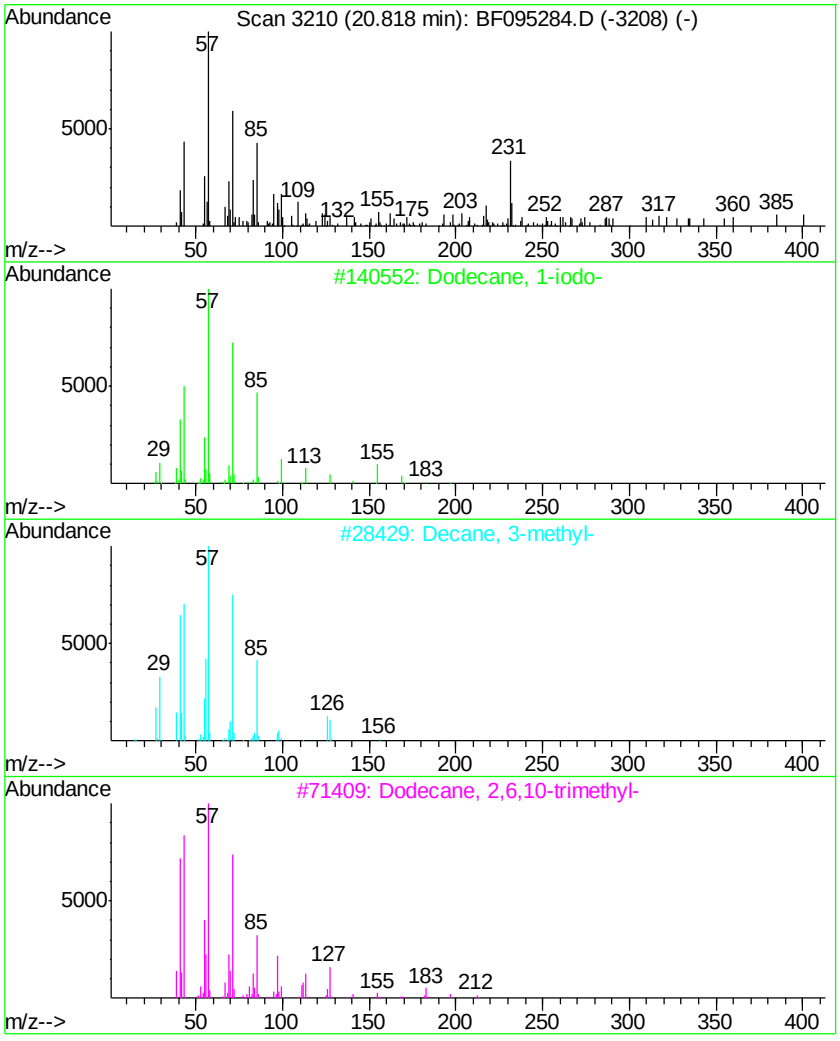
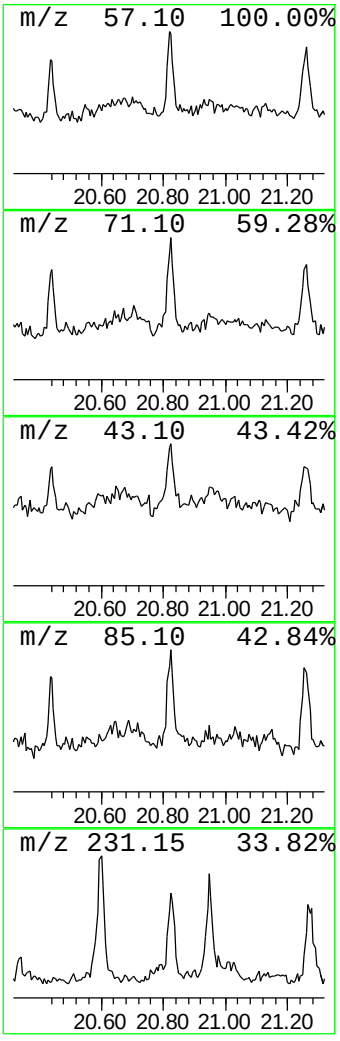
Peak Number 9 unknown20.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	5.20 ng	101075	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
2	Decane, 3-methyl-	156	C11H24	013151-34-3	38
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	38
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38
5	Tetradecane	198	C14H30	000629-59-4	35





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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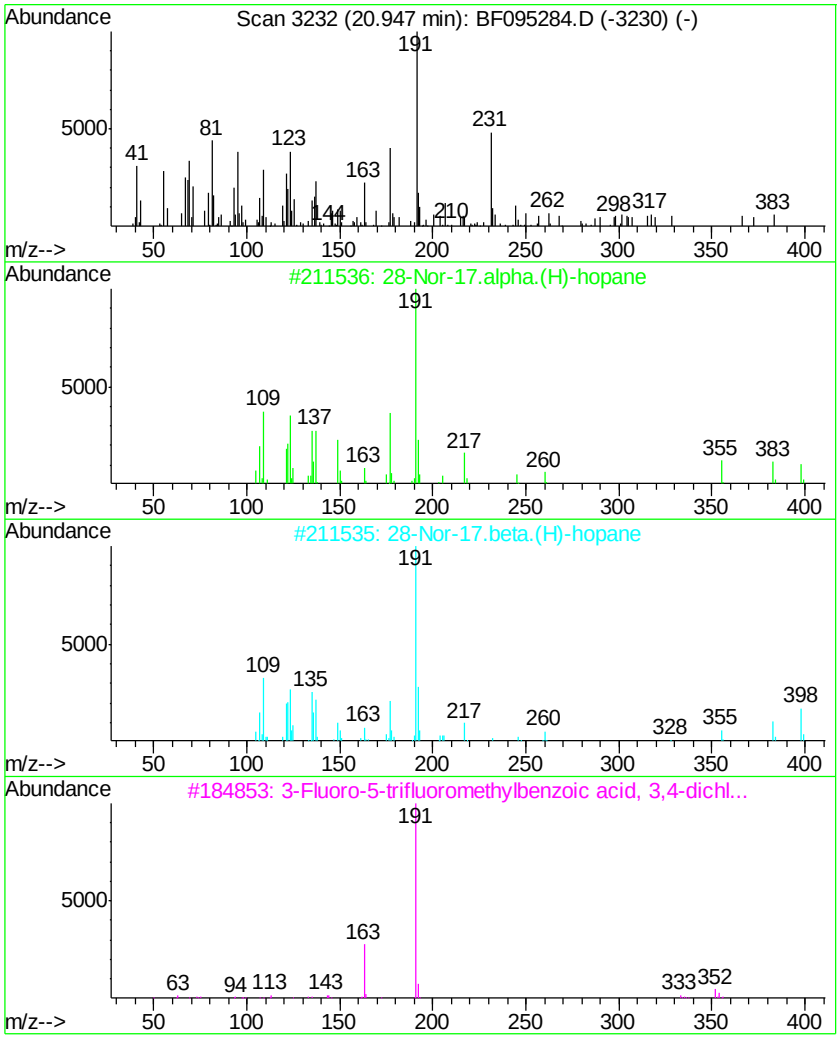
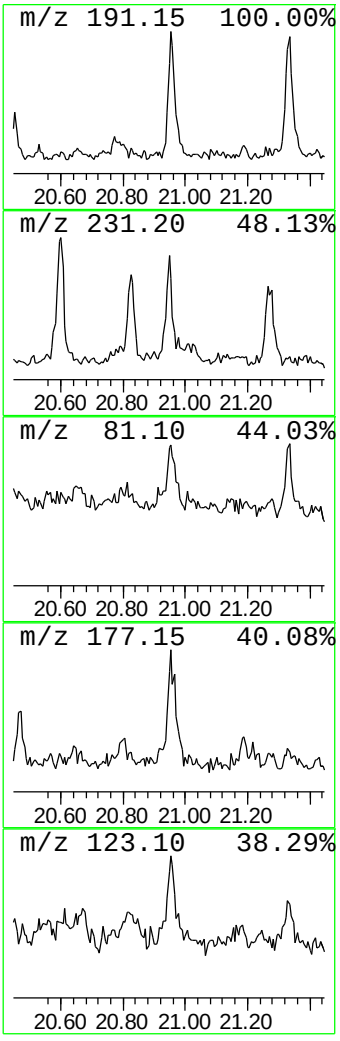
Peak Number 10 28-Nor-17.alpha.(H)-hopane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	8.38 ng	162859	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	68
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	64
3	3-Fluoro-5-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-96-2	38
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	37
5	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	37





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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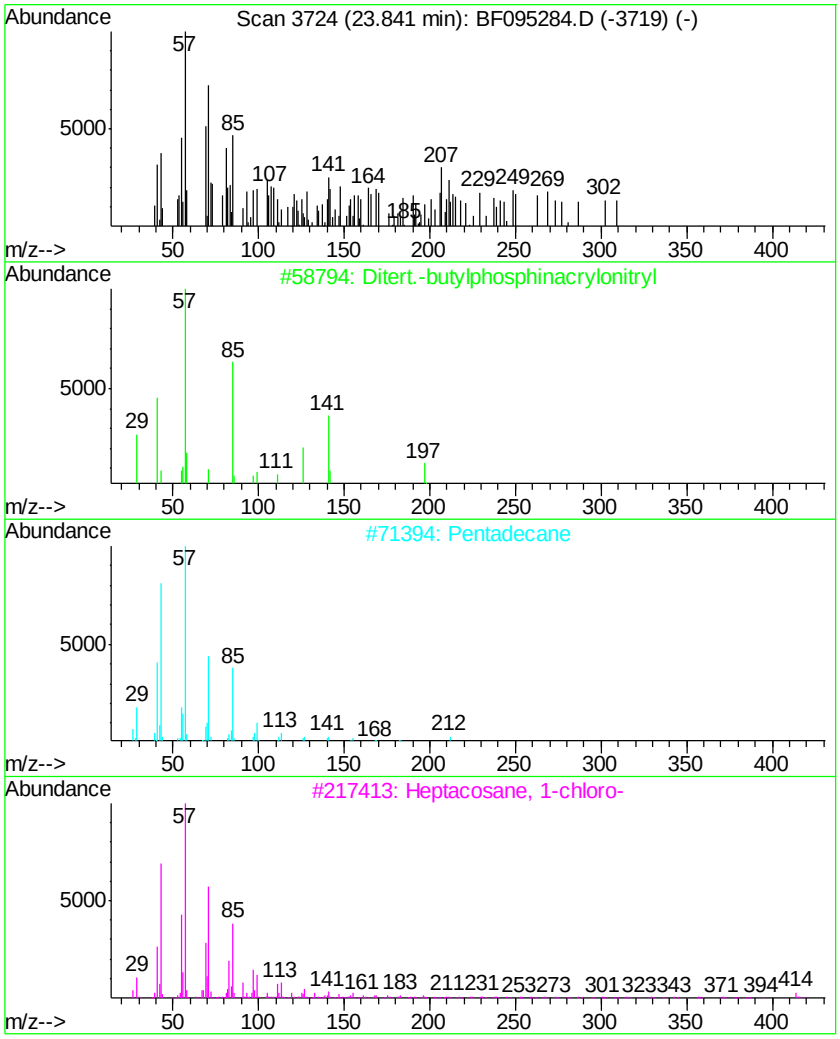
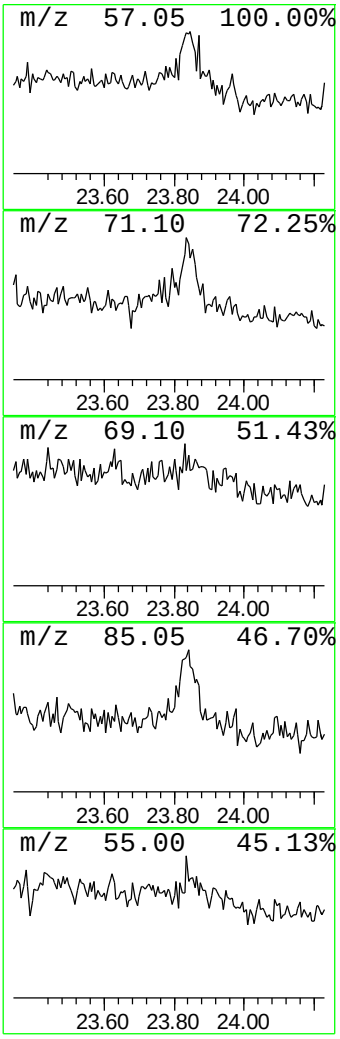
Peak Number 11 unknown23.84 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.84	2.30 ng	44740	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ditert.-butylphosphinacrylonitryl	197	C11H20NP	077376-95-5	18
2	Pentadecane	212	C15H32	000629-62-9	18
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	18
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	18
5	Sulfurous acid, pentyl tetradecy...	348	C19H40O3S	1000309-14-7	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095284.D
Acq On : 20 May 2017 2:28
Operator : SJ/MA
Sample : I3189-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-13-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	11.2	ng	315662	1	7.76	566225	20.0
unknown7.42	7.42	78.3	ng	2216500	1	7.76	566225	20.0
n-Hexadecanoic acid	15.97	3.5	ng	105386	4	15.02	606341	20.0
9-Phenyl-5H-benzo...	17.72	2.0	ng	71282	5	18.69	709567	20.0
1-Dodecanol, 2-oc...	18.58	3.0	ng	105950	5	18.69	709567	20.0
unknown20.82	20.82	5.2	ng	101075	6	20.37	388455	20.0
28-Nor-17.alpha.(...	20.95	8.4	ng	162859	6	20.37	388455	20.0
unknown23.84	23.84	2.3	ng	44740	6	20.37	388455	20.0