LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085872.D
Acq On : 30 Mar 2016 2:09
Operator : UM/SJ
Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

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-BF032416.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	4.321	176	178	186	rVB2	11789	24663	1.01%	0.093%
2	4.996	234	237	245	rBV	51721	86195	3.53%	0.327%
3	5.407	270	273	275	rBV	2392581	2422591	99.17%	9.178%
4	6.447	362	364	367	rBV	2026322	2247568	92.00%	8.515%
5	6.573	373	375	378	rBV	2318060	2294665	93.93%	8.693%
6	6.802	393	395	398	rBV	651256	662470	27.12%	2.510%
7	6.962	407	409	412	rBV	2247132	1979385	81.02%	7.499%
8	7.373	442	445	447	rBV	1655855	1507053	61.69%	5.709%
9	7.476	451	454	461	rVB	34712	50386	2.06%	0.191%
10	8.093	505	508	510	rBV	1041848	891674	36.50%	3.378%
11	9.167	600	602	605	rBV	2438399	2442989	100.00%	9.255%
12	9.568	635	637	639	rBV	409888	345946	14.16%	1.311%
13	9.785	653	656	658	rVV	36936	44391	1.82%	0.168%
14	9.842	659	661	663	rVV	640585	756556	30.97%	2.866%
15	9.876	663	664	667	rVB	35146	31760	1.30%	0.120%
16	10.253	695	697	698	rBV	24108	24580	1.01%	0.093%
17	10.276	698	699	701	rVB	75687	63849	2.61%	0.242%
18	10.505	716	719	722	rBV	22500	45507	1.86%	0.172%
19	10.630	728	730	733	rBV2	963997	1201284	49.17%	4.551%
20	10.756	739	741	747	rVB	68439	113230	4.63%	0.429%
21	10.939	756	757	762	rVB4	14406	26999	1.11%	0.102%
22	11.202	776	780	781	rBV3	51386	69699	2.85%	0.264%
23	11.225	781	782	786	rVB	33142	36407	1.49%	0.138%
24	11.328	789	791	792	rBV	769518	672989	27.55%	2.550%
25	11.408	795	798	800	rVB	74153	80541	3.30%	0.305%
26	11.568	809	812	815	rBV2	19466	31899	1.31%	0.121%
27	11.625	815	817	819	rVV	44461	35857	1.47%	0.136%
28	11.831	833	835	836	rBV	69806	59474	2.43%	0.225%
29	11.865	836	838	840	rVV2	171252	210285	8.61%	0.797%
30	11.911	840	842	843	rVV	32408	41125	1.68%	0.156%
31	11.945	843	845	849	rVB2	83063	140907	5.77%	0.534%
32	12.036	849	853	855	rBV3	12257	24678	1.01%	0.093%
33	12.128	857	861	862	rBV	53990	58334	2.39%	0.221%
34	12.151	862	863	865	rVB	29115	34597	1.42%	0.131%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

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-BF032416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.276	871	874	875	rBV	27844	36870	1.51%	0.140%
36	12.379	881	883	885	rBV	48165	59320	2.43%	0.225%
37	12.414	885	886	889	rVV2	34585	54314	2.22%	0.206%
38	12.471	889	891	895	rVB	49609	54071	2.21%	0.205%
39	12.539	895	897	900	rBV	707352	644016	26.36%	2.440%
40	12.642	904	906	908	rVV	38789	49382	2.02%	0.187%
41	12.688	908	910	912	rVB2	23780	34997	1.43%	0.133%
42	12.768	912	917	920	rBV	738685	768599	31.46%	2.912%
43	12.814	920	921	924	rVB2	27982	45855	1.88%	0.174%
44	12.916	927	930	932	rVV	2212515	2109553	86.35%	7.992%
45	12.985	933	936	938	rBV2	52158	97582	3.99%	0.370%
46	13.099	942	946	947	rVB	58958	118710	4.86%	0.450%
47	13.145	947	950	951	rBV2	22926	40991	1.68%	0.155%
48	13.202	953	955	959	rBV2	78069	107122	4.38%	0.406%
49	13.294	961	963	964	rBV	51002	40241	1.65%	0.152%
50	13.328	964	966	967	rBV	34102	37454	1.53%	0.142%
51	13.488	977	980	981	rBV2	20594	31481	1.29%	0.119%
52	13.602	989	990	992	rBV	59494	72561	2.97%	0.275%
53	13.717	997	1000	1001	rBV	70940	92747	3.80%	0.351%
54	13.762	1003	1004	1007	rVV2	44328	82292	3.37%	0.312%
55	13.819	1007	1009	1011	rVB	113936	162203	6.64%	0.614%
56	13.968	1019	1022	1023	rBV2	829063	1051884	43.06%	3.985%
57	14.071	1029	1031	1032	rBV2	45763	45551	1.86%	0.173%
58	14.357	1054	1056	1057	rVB	46866	45567	1.87%	0.173%
59	14.711	1085	1087	1090	rBV3	42496	64663	2.65%	0.245%
60	14.985	1108	1111	1115	rBV	240168	446815	18.29%	1.693%
61	15.271	1134	1136	1139	rVB	113184	142590	5.84%	0.540%
62	15.328	1139	1141	1144	rVB	193302	222993	9.13%	0.845%
63	15.385	1144	1146	1152	rBV	434708	607626	24.87%	2.302%
64	16.768	1264	1267	1270	rBV	58737	114409	4.68%	0.433%
65	17.180	1301	1303	1312	rVB	54575	153425	6.28%	0.581%

Sum of corrected areas: 26396417

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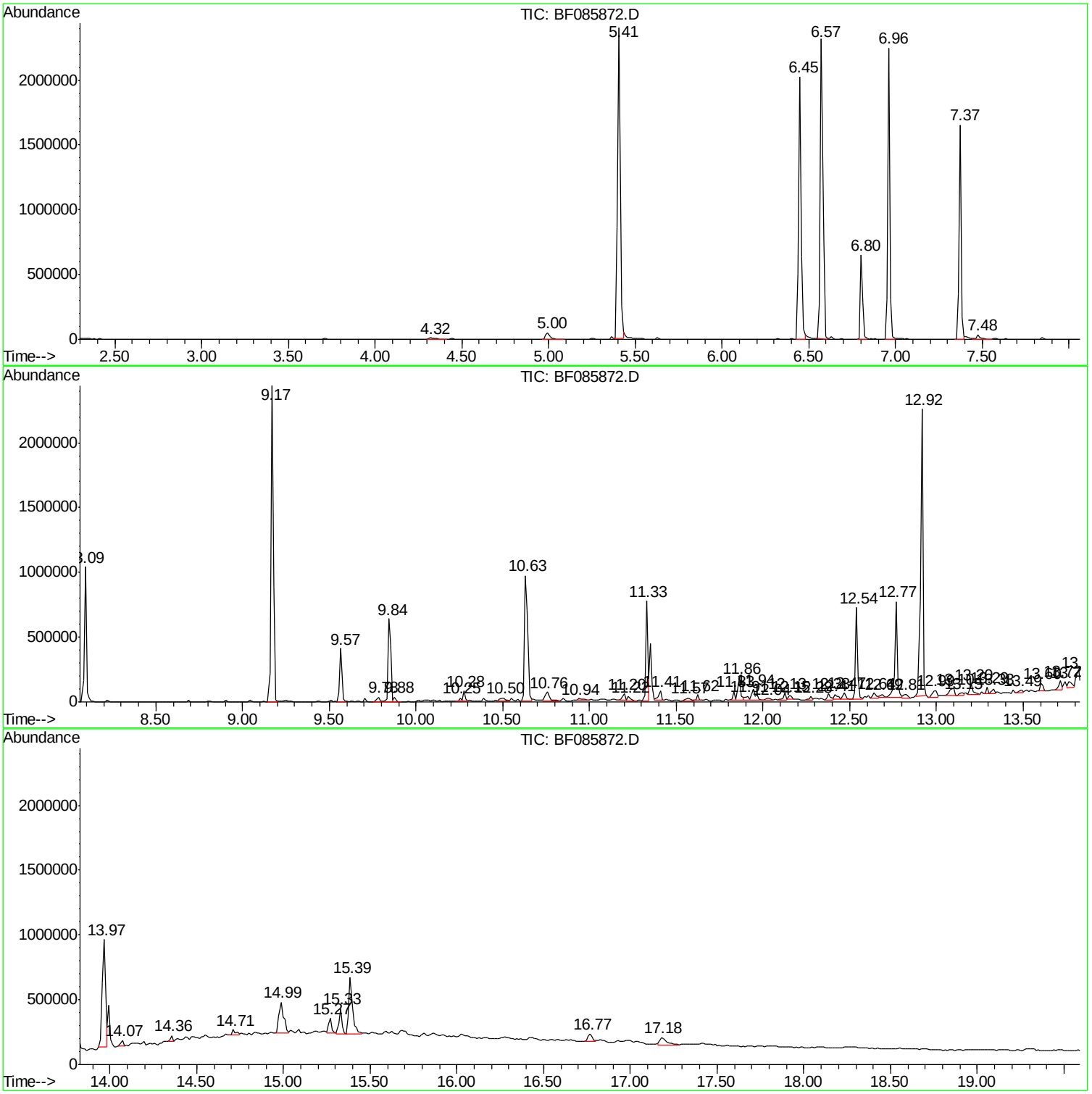
Instrument :
BNA_F
ClientSampleId :
NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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

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Data File : BF085872.D
Acq On : 30 Mar 2016 2:09
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Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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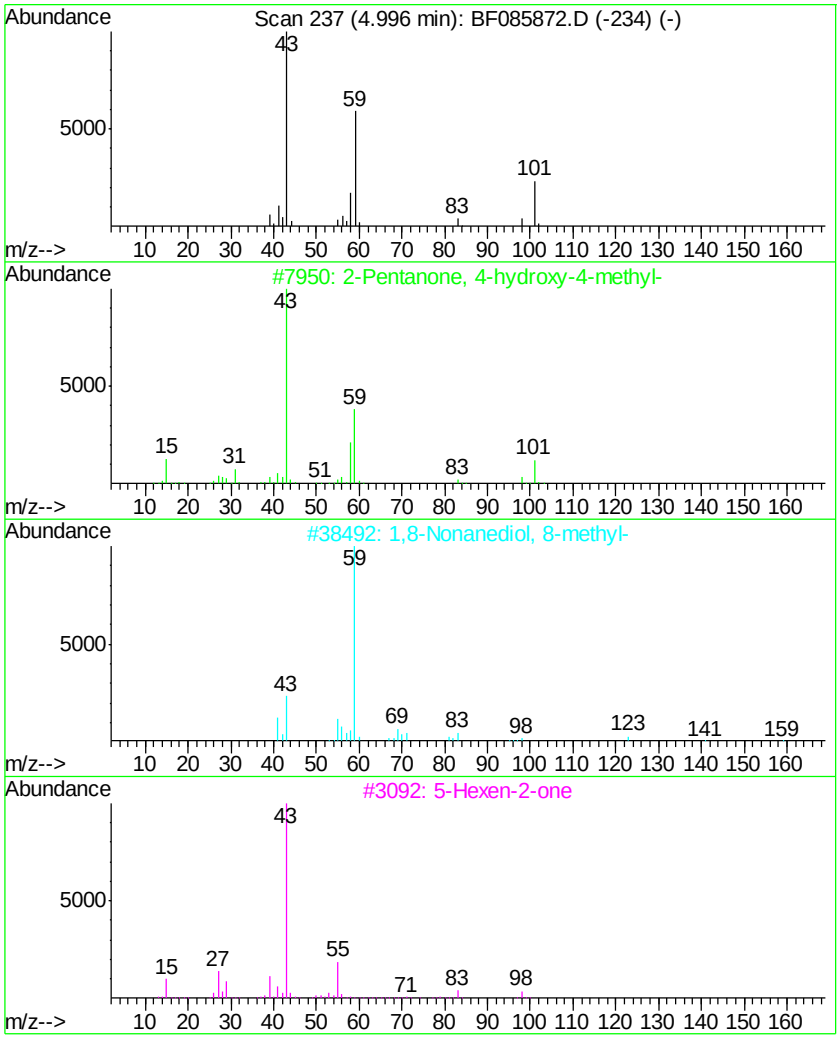
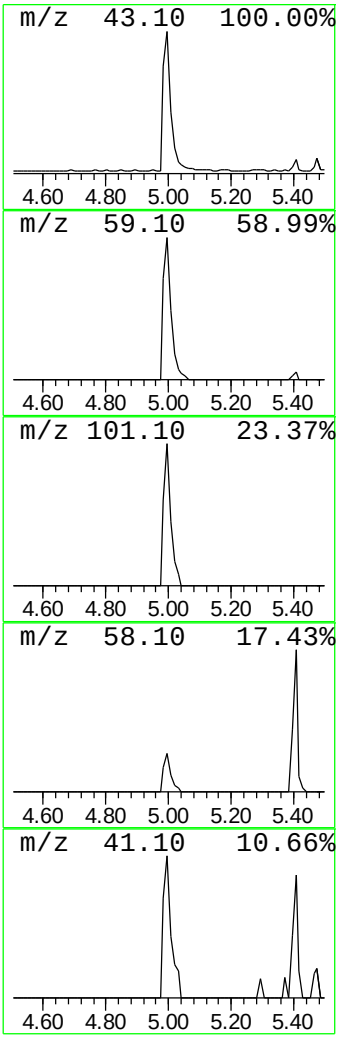
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.60 ng	86195	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	56
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : H1978-02
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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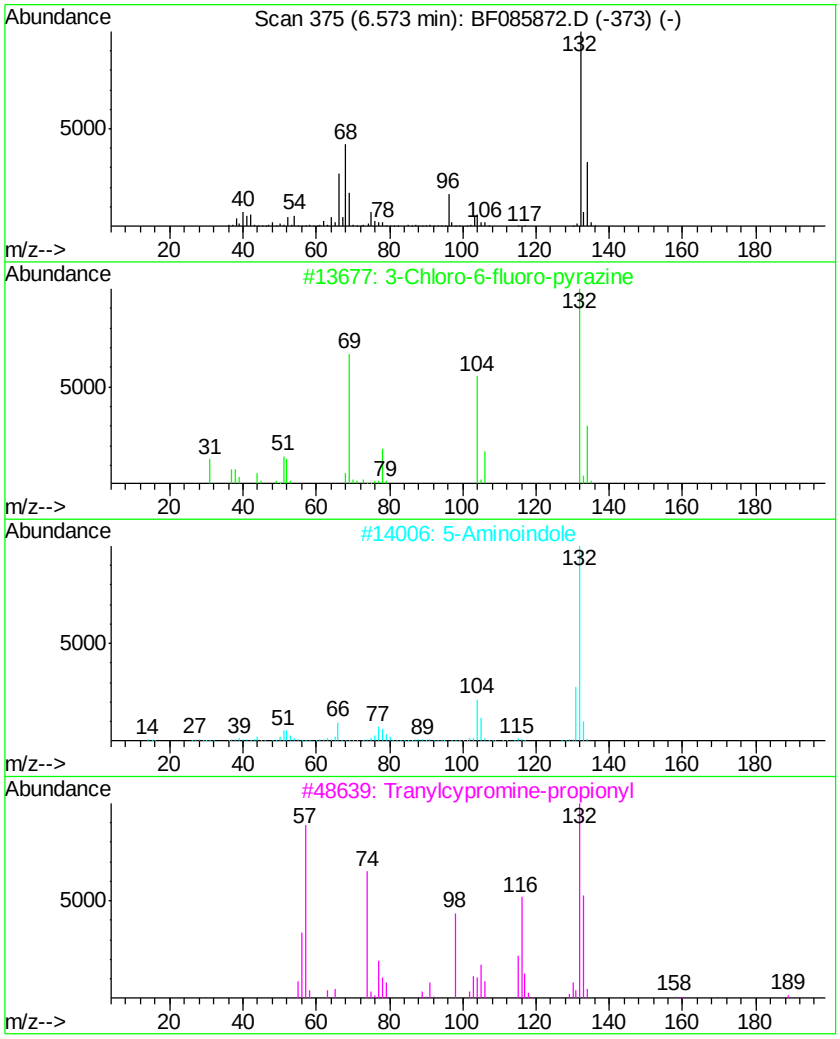
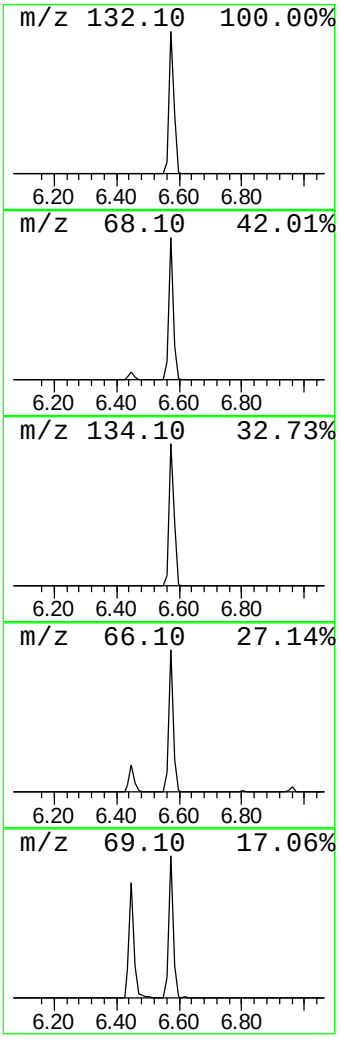
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	69.28 ng	2294670	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	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
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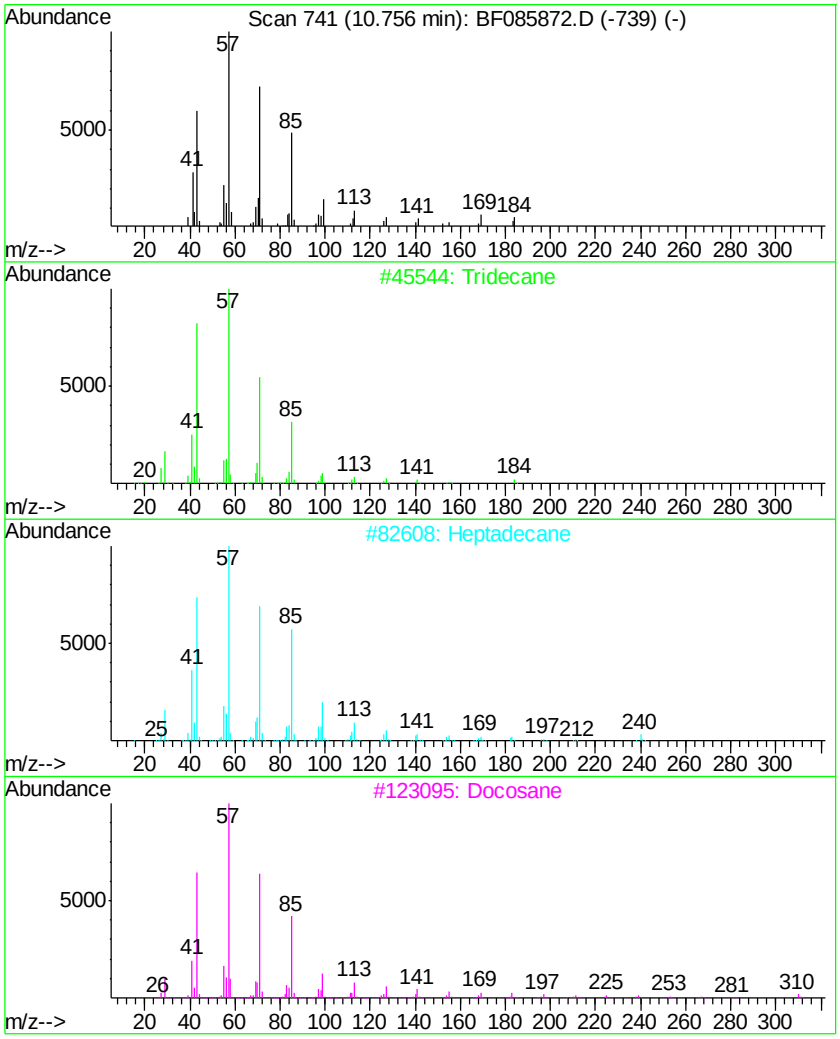
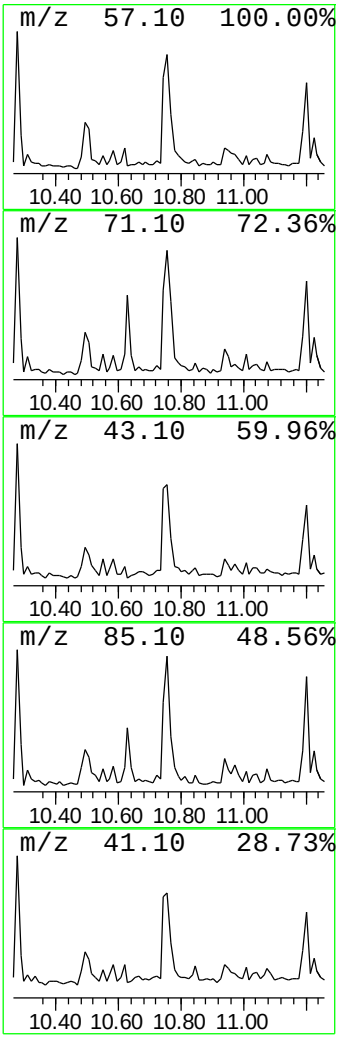
Peak Number 4 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	3.36 ng	113230	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Heptadecane	240	C17H36	000629-78-7	90
3	Docosane	310	C22H46	000629-97-0	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87





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Sample : H1978-02
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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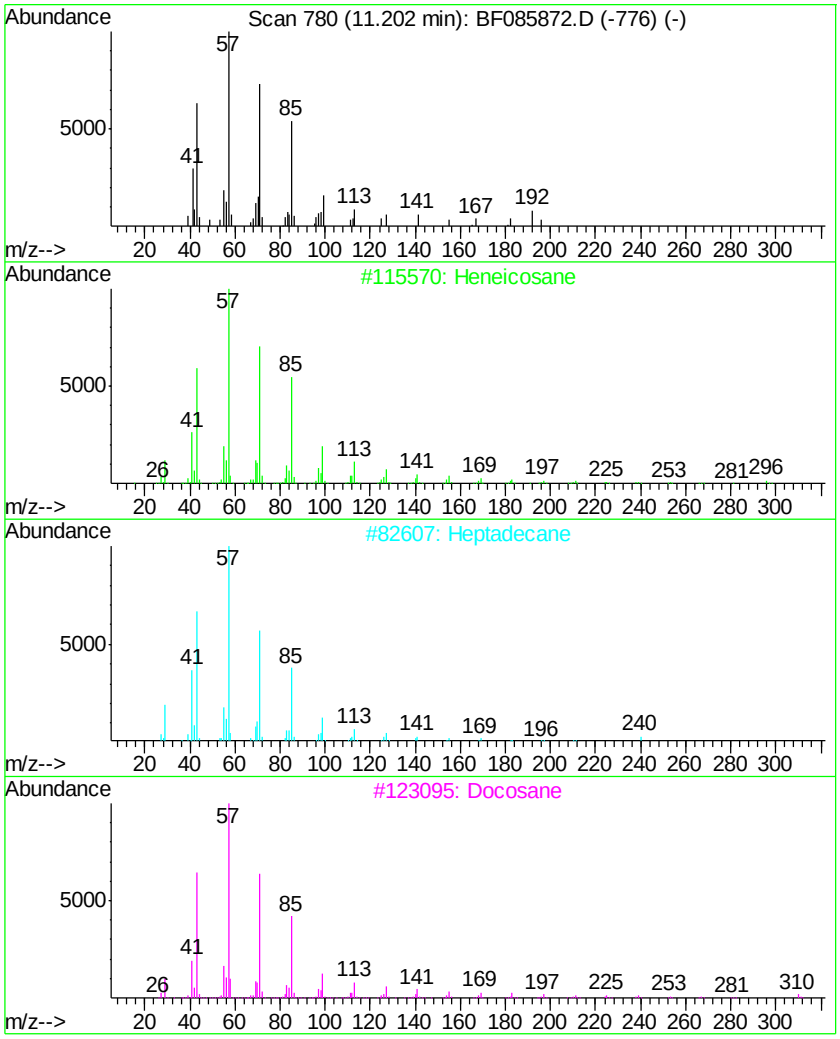
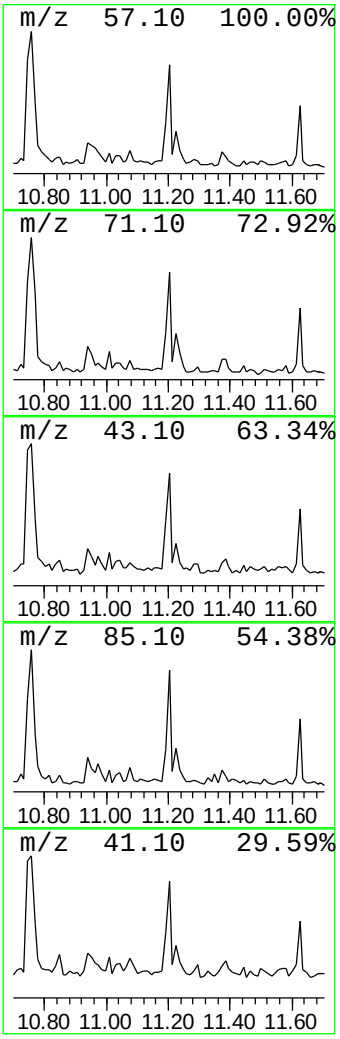
Peak Number 5 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.07 ng	69699	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane	240	C17H36	000629-78-7	80
3	Docosane	310	C22H46	000629-97-0	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Nonacosane	408	C29H60	000630-03-5	80





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Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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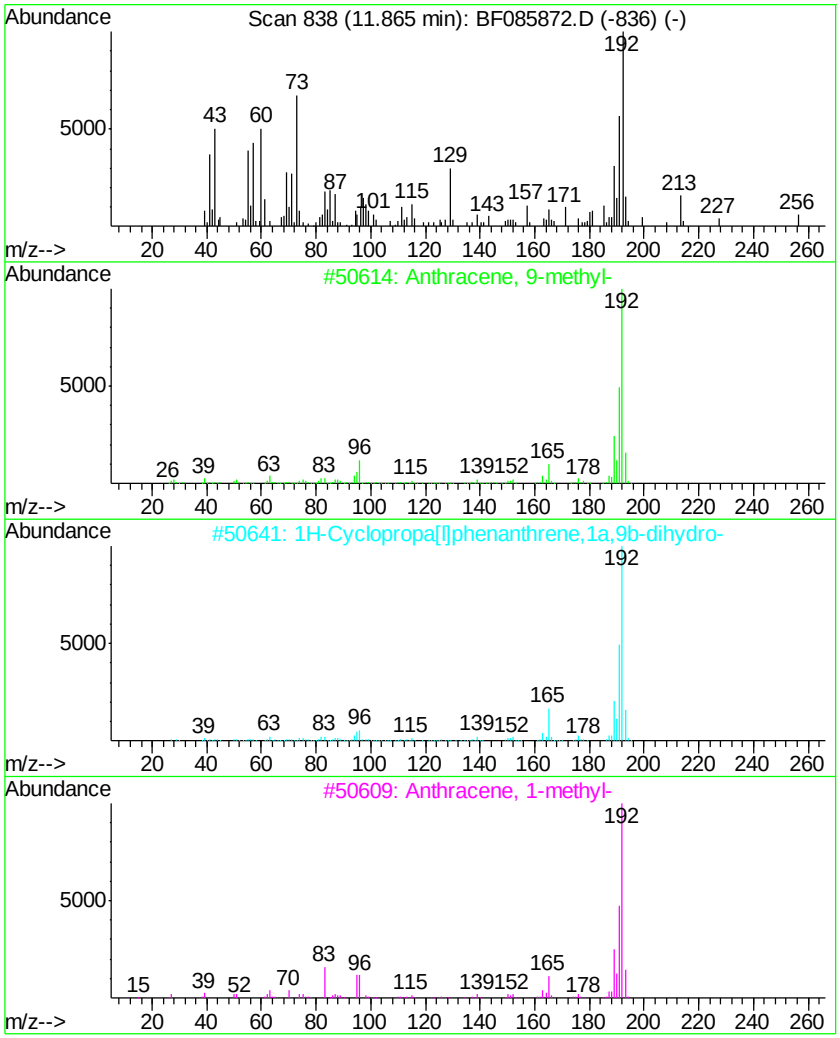
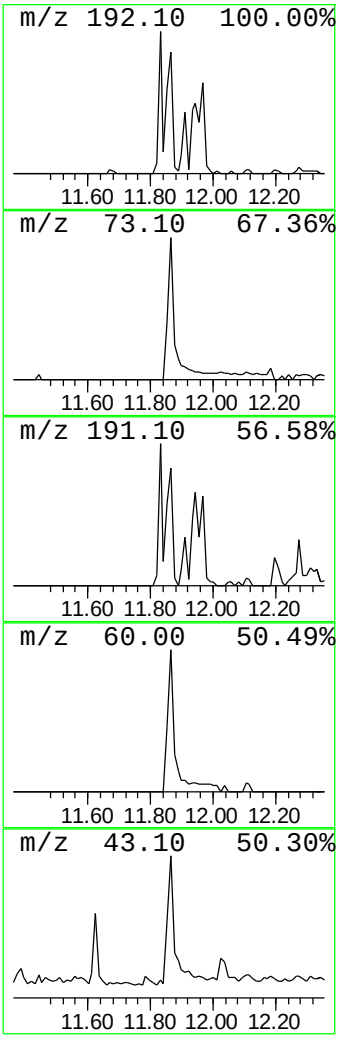
Peak Number 6 Anthracene, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	6.25 ng	210285	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	92
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	78
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	62





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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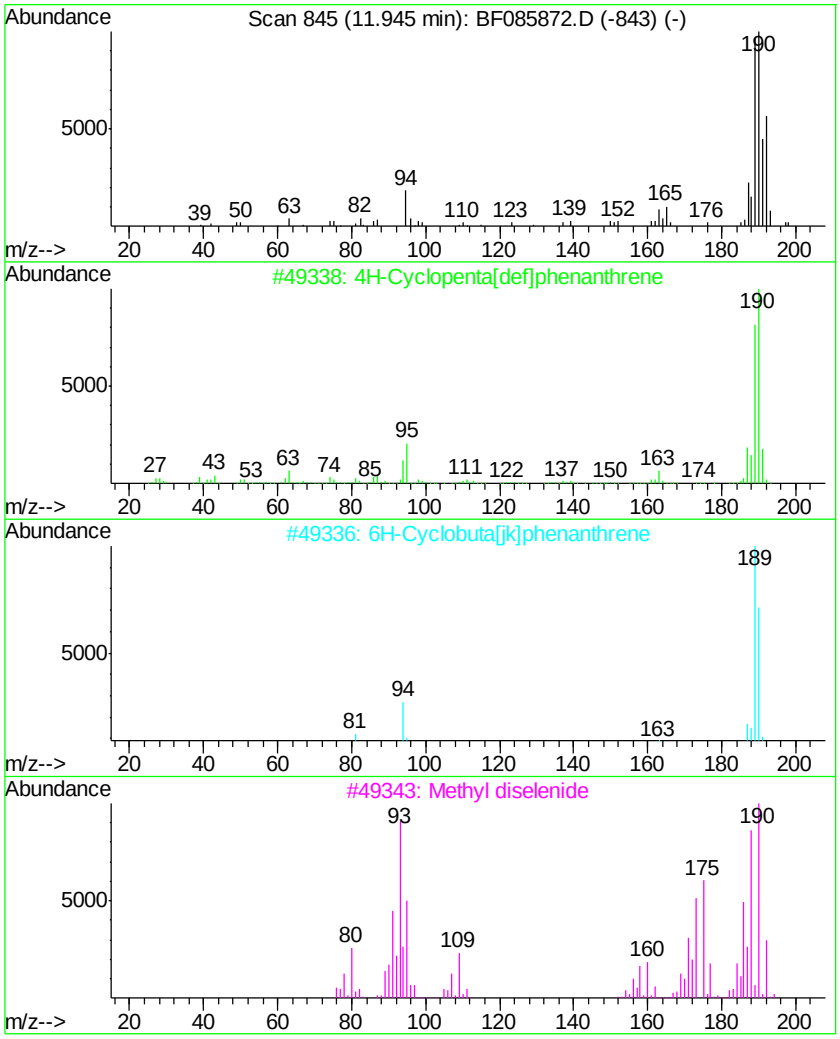
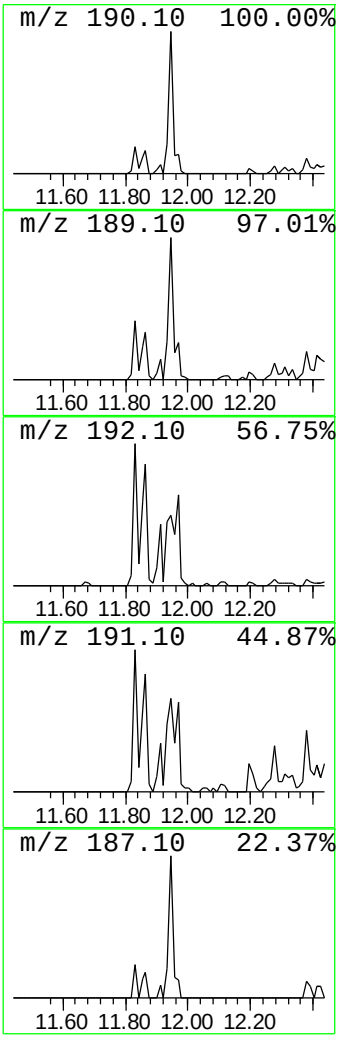
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.19 ng	140907	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	41
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	25





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Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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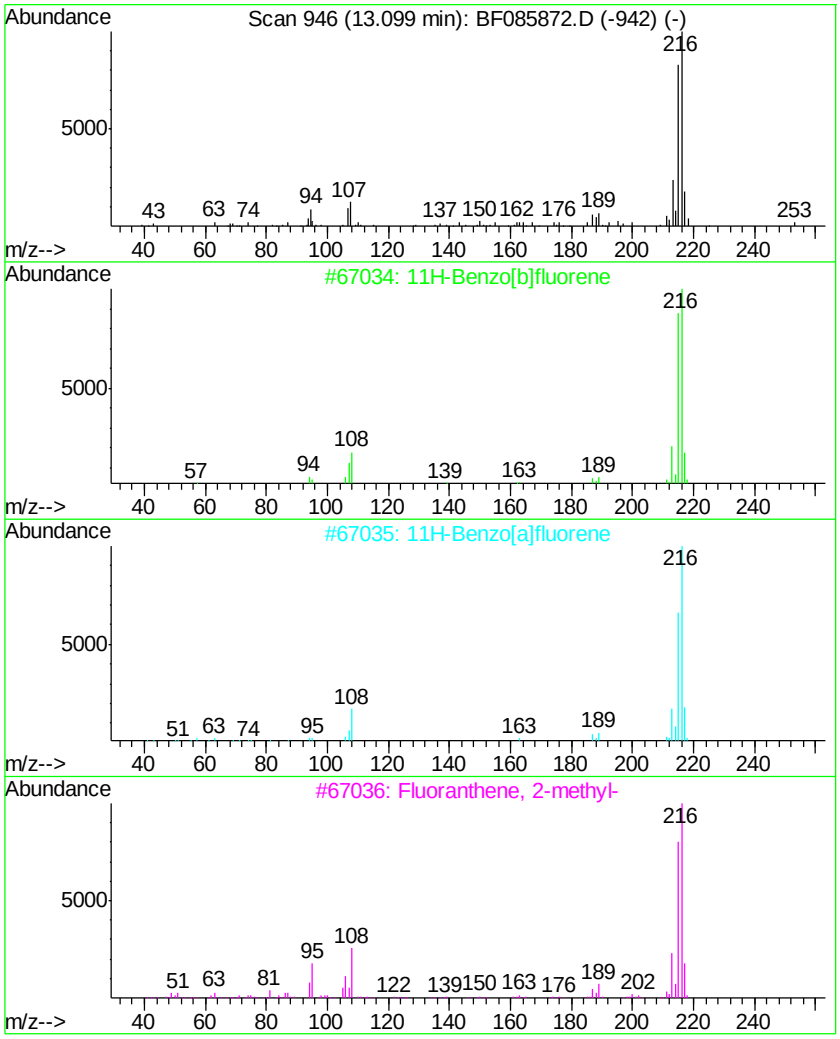
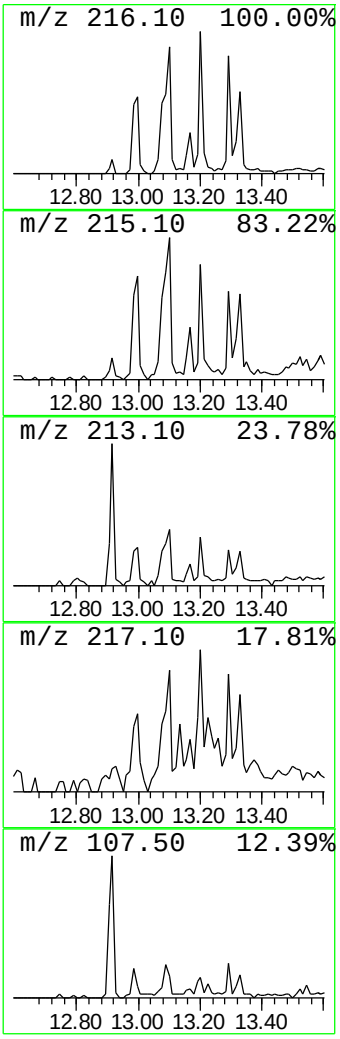
Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.26 ng	118710	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032916\
Data File : BF085872.D
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Operator : UM/SJ
Sample : H1978-02
Misc :
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Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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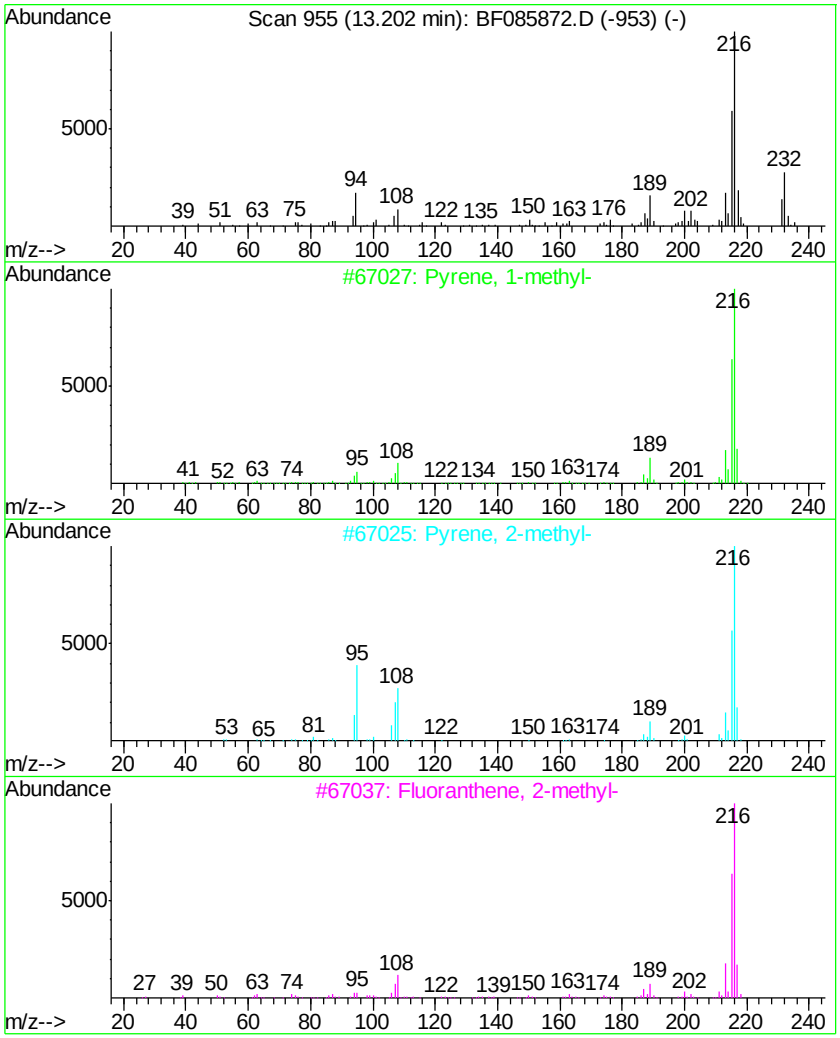
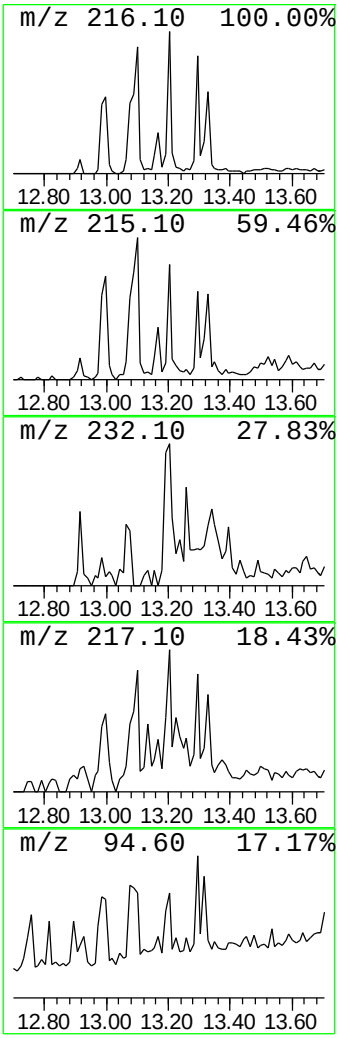
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	2.04 ng	107122	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	89
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	70





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Acq On : 30 Mar 2016 2:09
Operator : UM/SJ
Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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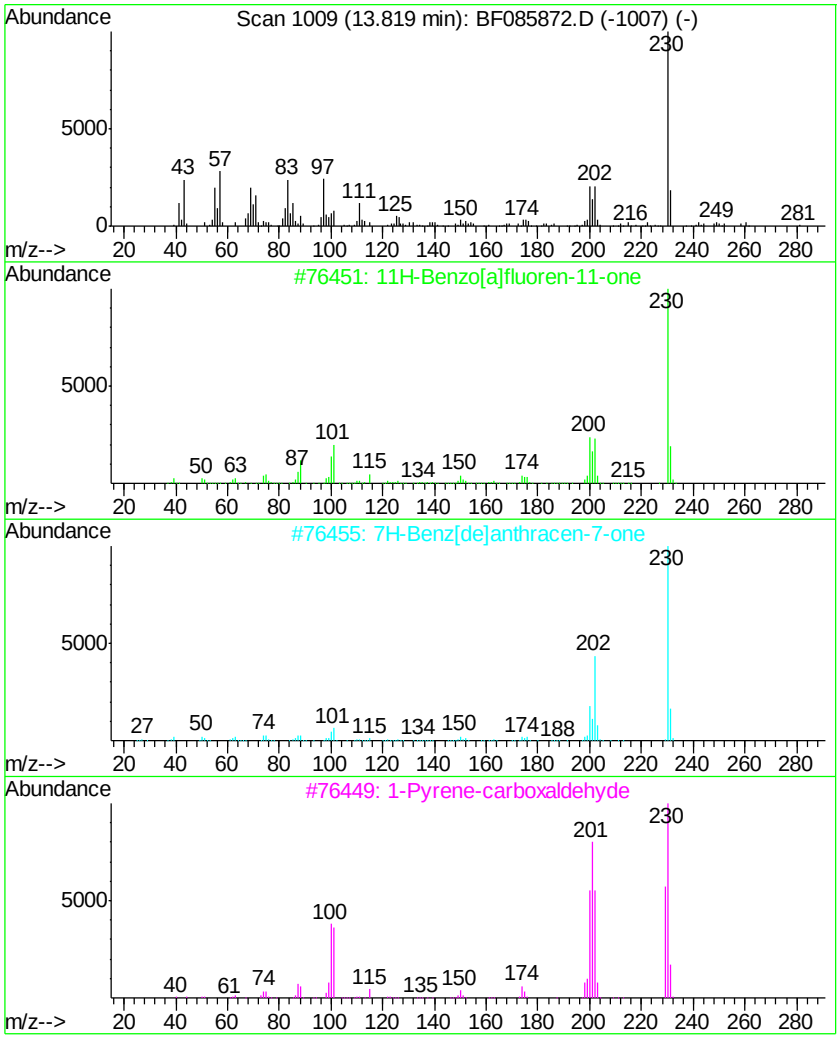
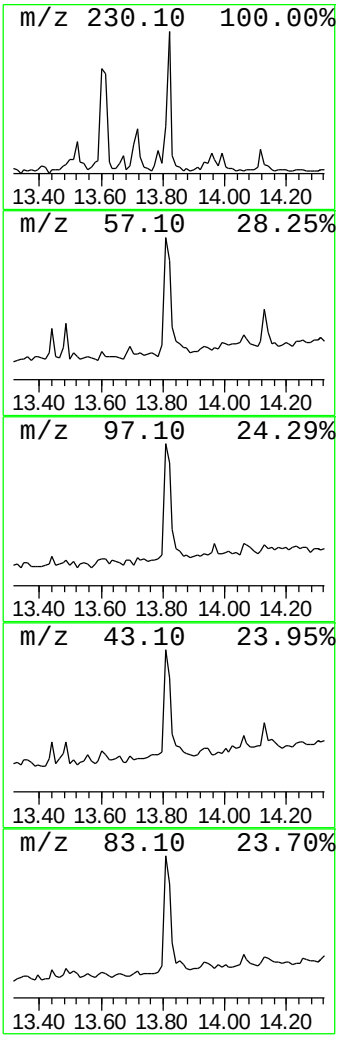
Peak Number 10 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.08 ng	162203	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	78
3	1-Pyrene-carboxaldehyde	230	C17H10O	003029-19-4	40
4	p-Terphenyl	230	C18H14	000092-94-4	38
5	Ethyl 5-(p-tolyl)pyrazole-3-carb...	230	C13H14N2O2	1000211-61-7	35





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Sample : H1978-02
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
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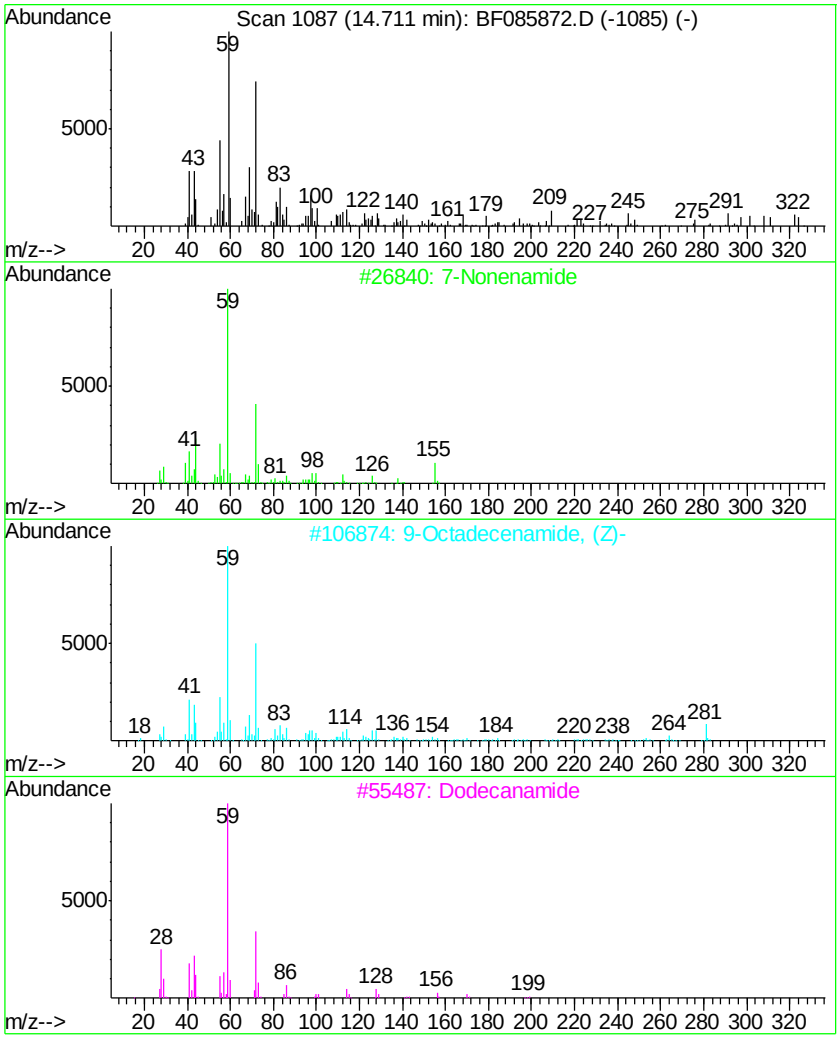
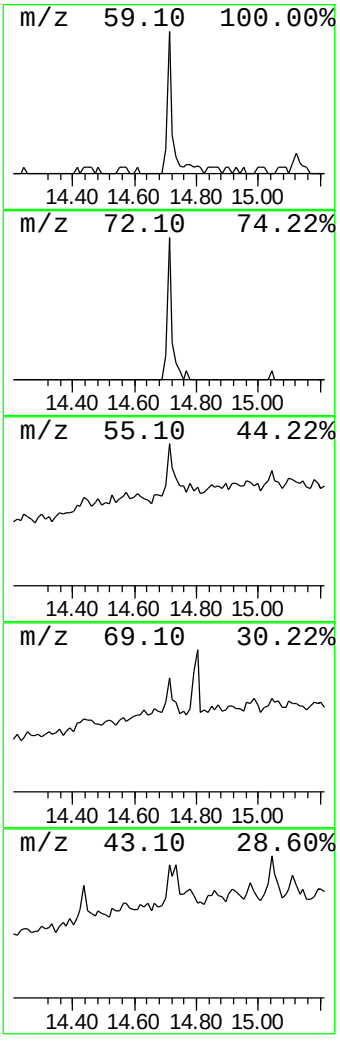
Peak Number 11 unknown14.71 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.13 ng	64663	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide	155	C9H17NO	090949-53-4	47
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	47
3	Dodecanamide	199	C12H25NO	001120-16-7	45
4	Pentanamide	101	C5H11NO	000626-97-1	35
5	Hexadecanamide	255	C16H33NO	000629-54-9	32





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Data File : BF085872.D
Acq On : 30 Mar 2016 2:09
Operator : UM/SJ
Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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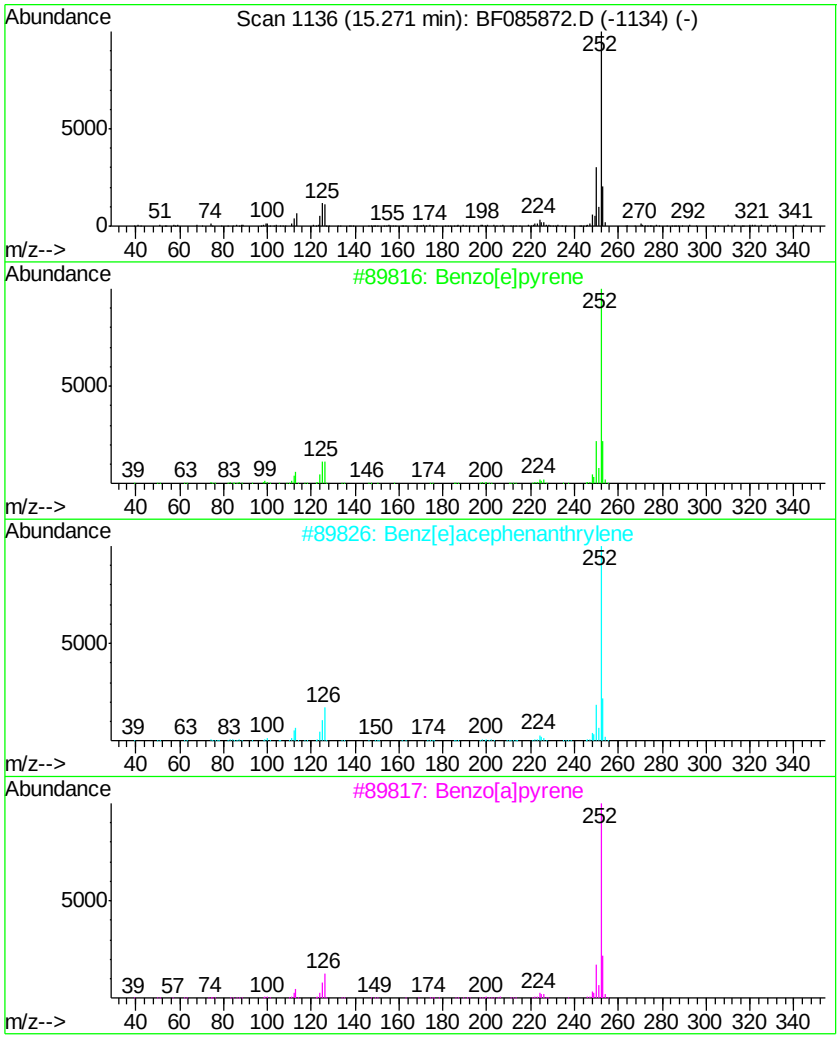
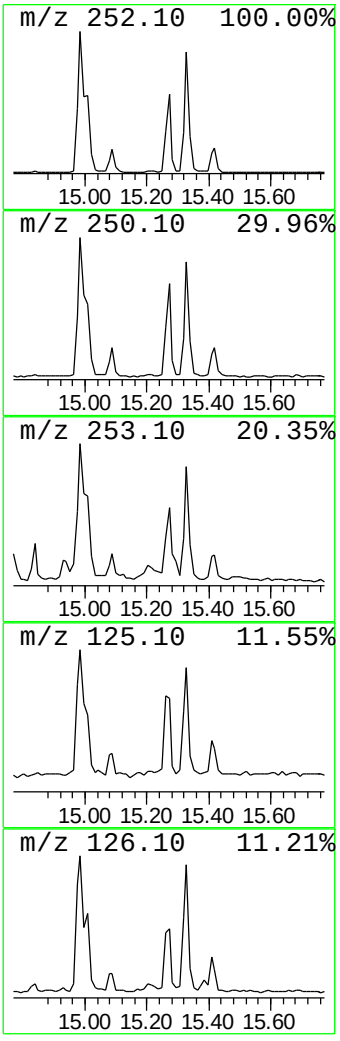
Peak Number 12 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	4.69 ng	142590	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





Tentatively Identified Compound (LSC) summary

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Data File : BF085872.D
Acq On : 30 Mar 2016 2:09
Operator : UM/SJ
Sample : H1978-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCB-083-CS-2(0-7FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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...	5.00	2.6	ng	86195	1	6.80	662470	20.0
unknown6.57	6.57	69.3	ng	2294670	1	6.80	662470	20.0
Tridecane	10.76	3.4	ng	113230	4	11.33	672989	20.0
Heneicosane	11.20	2.1	ng	69699	4	11.33	672989	20.0
Anthracene, 9-met...	11.86	6.3	ng	210285	4	11.33	672989	20.0
4H-Cyclopenta[def...	11.94	4.2	ng	140907	4	11.33	672989	20.0
11H-Benzo[b]fluorene	13.10	2.3	ng	118710	5	13.97	1051880	20.0
Pyrene, 1-methyl-	13.20	2.0	ng	107122	5	13.97	1051880	20.0
11H-Benzo[a]fluor...	13.82	3.1	ng	162203	5	13.97	1051880	20.0
unknown14.71	14.71	2.1	ng	64663	6	15.39	607626	20.0
Benzo[e]pyrene	15.27	4.7	ng	142590	6	15.39	607626	20.0