LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095692.D
Acq On : 6 Jun 2017 1:22
Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

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-BF060517.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	1.601	8	11	33	rBV	481857	927444	43.84%	4.344%
2	4.613	519	523	538	rBV	56096	145430	6.87%	0.681%
3	5.295	635	639	668	rBV	1077081	1894307	89.54%	8.874%
4	6.954	917	921	933	rBV	1202178	1777531	84.02%	8.327%
5	7.054	933	938	955	rVB	1413125	1945566	91.96%	9.114%
6	7.395	992	996	1013	rVB	384805	507615	23.99%	2.378%
7	7.636	1032	1037	1059	rBV	1110566	1435813	67.86%	6.726%
8	8.313	1147	1152	1168	rBV	863478	1224499	57.88%	5.736%
9	9.430	1337	1342	1358	rBV	501941	672148	31.77%	3.149%
10	10.595	1536	1540	1550	rVB	31453	43687	2.06%	0.205%
11	10.742	1559	1565	1573	rBV	53483	70292	3.32%	0.329%
12	11.207	1638	1644	1654	rBV	1740917	2115713	100.00%	9.911%
13	11.501	1691	1694	1705	rVB3	11418	23891	1.13%	0.112%
14	11.607	1709	1712	1721	rBV4	32992	67489	3.19%	0.316%
15	11.730	1727	1733	1737	rBV	60629	83329	3.94%	0.390%
16	11.771	1737	1740	1747	rVB	33627	43702	2.07%	0.205%
17	11.901	1757	1762	1771	rBV	283331	378973	17.91%	1.775%
18	12.042	1780	1786	1792	rBV2	25167	38067	1.80%	0.178%
19	12.248	1816	1821	1826	rBV2	551222	674560	31.88%	3.160%
20	12.301	1826	1830	1836	rVB3	33378	51813	2.45%	0.243%
21	12.460	1852	1857	1863	rBV3	11527	21243	1.00%	0.100%
22	12.683	1889	1895	1899	rBV2	20328	27558	1.30%	0.129%
23	12.795	1910	1914	1921	rVB3	19966	29512	1.39%	0.138%
24	13.142	1970	1973	1979	rVB	57685	70277	3.32%	0.329%
25	13.230	1983	1988	1991	rBV5	14075	21880	1.03%	0.102%
26	13.542	2036	2041	2059	rVB	713543	927456	43.84%	4.345%
27	13.883	2093	2099	2105	rBV2	27364	52343	2.47%	0.245%
28	14.083	2130	2133	2139	rVB	19076	24149	1.14%	0.113%
29	14.477	2196	2200	2206	rVB	23225	29683	1.40%	0.139%
30	14.606	2218	2222	2224	rBV	18779	23069	1.09%	0.108%
31	14.642	2224	2228	2231	rVV	468385	577305	27.29%	2.704%
32	14.677	2231	2234	2244	rVV	212433	275021	13.00%	1.288%
33	14.771	2247	2250	2256	rVB	33893	45140	2.13%	0.211%
34	15.183	2316	2320	2324	rVB	22156	26614	1.26%	0.125%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.442	2360	2364	2368	rBV2	91802	110202	5.21%	0.516%
36	15.489	2368	2372	2377	rVB	69437	80996	3.83%	0.379%
37	15.595	2386	2390	2394	rVV2	83073	116059	5.49%	0.544%
38	15.653	2394	2400	2410	rVB2	106791	200478	9.48%	0.939%
39	15.895	2437	2441	2446	rBV3	24993	34612	1.64%	0.162%
40	16.253	2496	2502	2506	rBV	48613	67772	3.20%	0.317%
41	16.295	2506	2509	2513	rVV3	30771	40654	1.92%	0.190%
42	16.377	2518	2523	2525	rVV2	32966	44438	2.10%	0.208%
43	16.412	2525	2529	2532	rVV	103684	119988	5.67%	0.562%
44	16.453	2532	2536	2542	rVV	218135	311658	14.73%	1.460%
45	16.565	2551	2555	2562	rBV6	14692	37483	1.77%	0.176%
46	16.759	2583	2588	2593	rBV	206546	257752	12.18%	1.207%
47	17.012	2626	2631	2638	rVB	1202287	1408303	66.56%	6.597%
48	17.083	2638	2643	2646	rBV3	24237	34063	1.61%	0.160%
49	17.230	2659	2668	2673	rVB2	43015	89097	4.21%	0.417%
50	17.318	2675	2683	2686	rBV2	30588	56776	2.68%	0.266%
51	17.365	2686	2691	2696	rBV3	35391	58701	2.77%	0.275%
52	17.477	2706	2710	2713	rBV	26652	31636	1.50%	0.148%
53	17.518	2713	2717	2719	rVV	24815	30431	1.44%	0.143%
54	17.571	2723	2726	2730	rBV6	15380	24917	1.18%	0.117%
55	18.030	2797	2804	2807	rBV3	31327	61588	2.91%	0.288%
56	18.265	2840	2844	2854	rBV2	92936	171523	8.11%	0.803%
57	18.347	2854	2858	2862	rBV2	524275	691888	32.70%	3.241%
58	18.383	2862	2864	2873	rVB	65903	110629	5.23%	0.518%
59	18.571	2891	2896	2897	rBV5	19960	29830	1.41%	0.140%
60	18.859	2943	2945	2950	rVB	25535	29352	1.39%	0.137%
61	18.900	2950	2952	2956	rVB2	22987	23578	1.11%	0.110%
62	19.618	3071	3074	3079	rBV	51495	87549	4.14%	0.410%
63	19.794	3100	3104	3108	rBV	139446	161363	7.63%	0.756%
64	19.912	3121	3124	3127	rBV	33403	34698	1.64%	0.163%
65	19.965	3131	3133	3137	rVV	52313	58478	2.76%	0.274%
66	20.018	3138	3142	3150	rVB	381046	458125	21.65%	2.146%

Sum of corrected areas: 21347736

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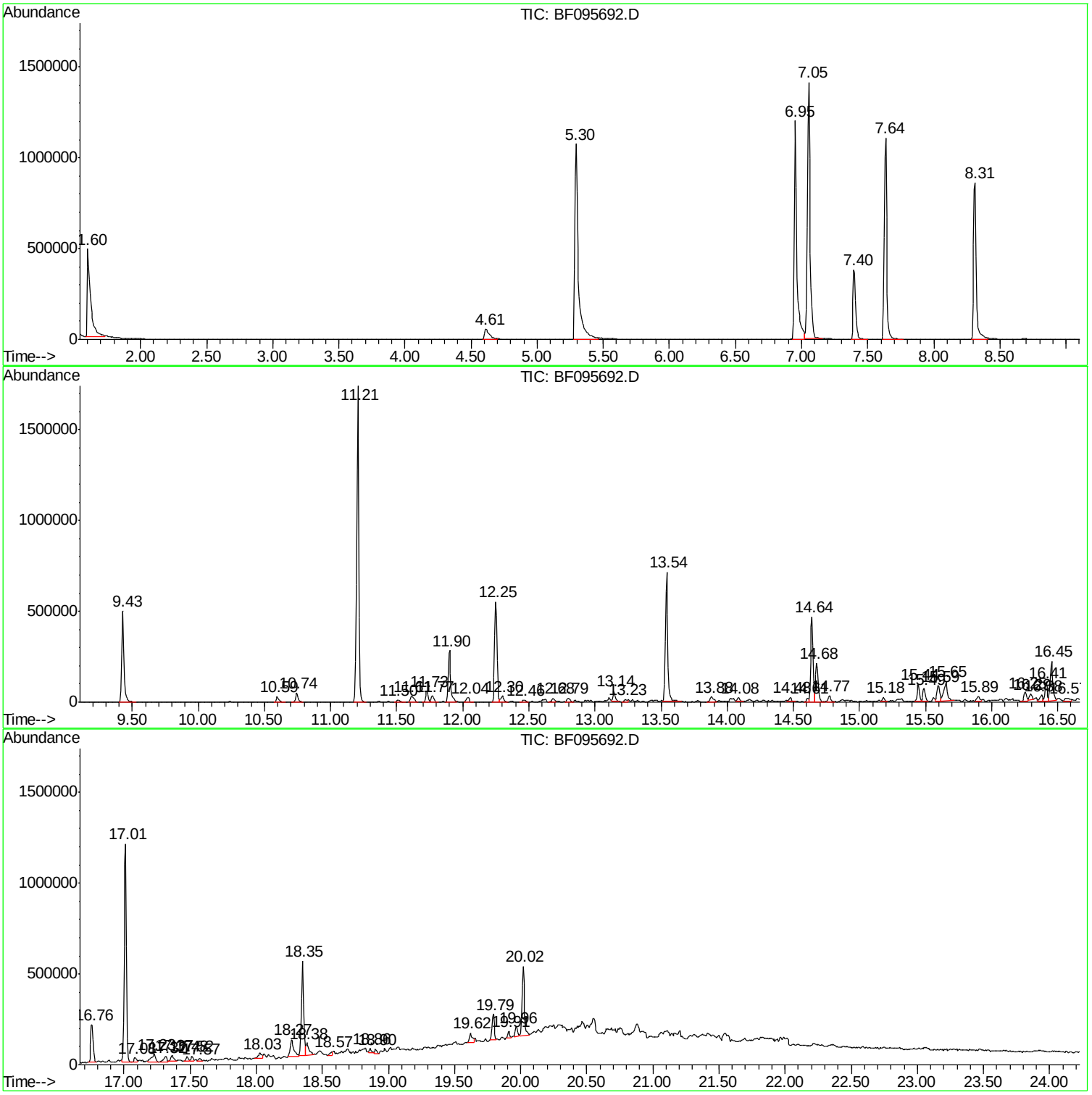
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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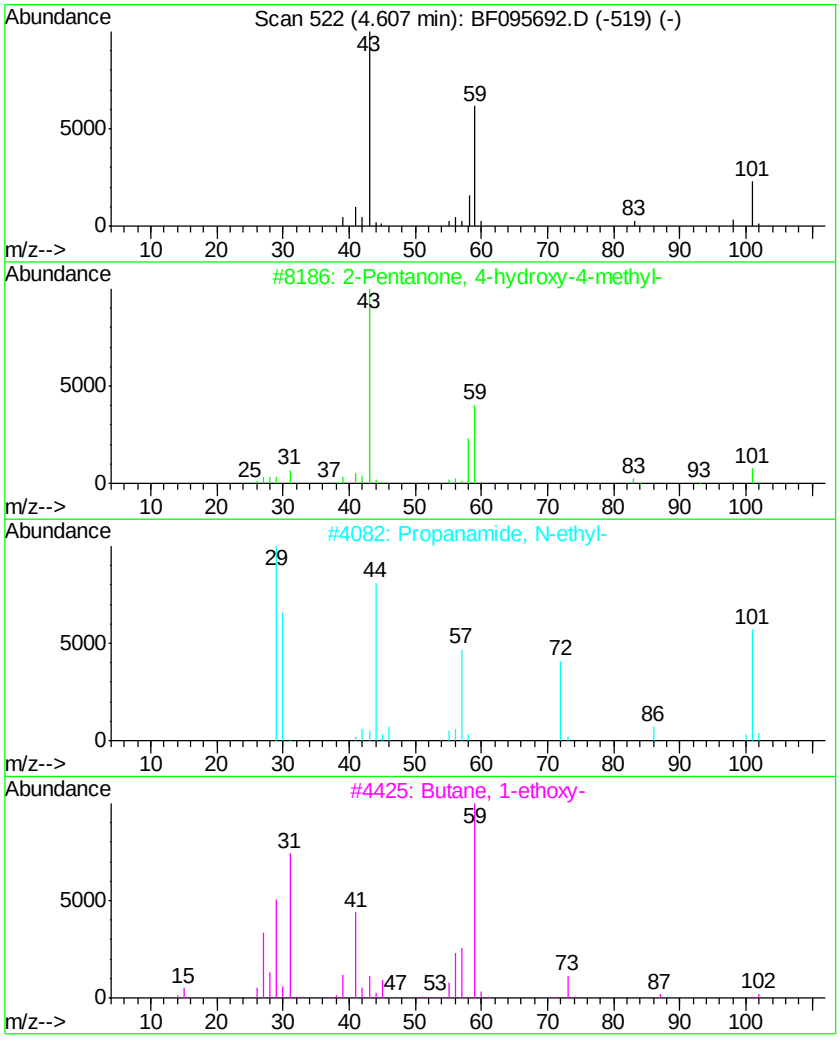
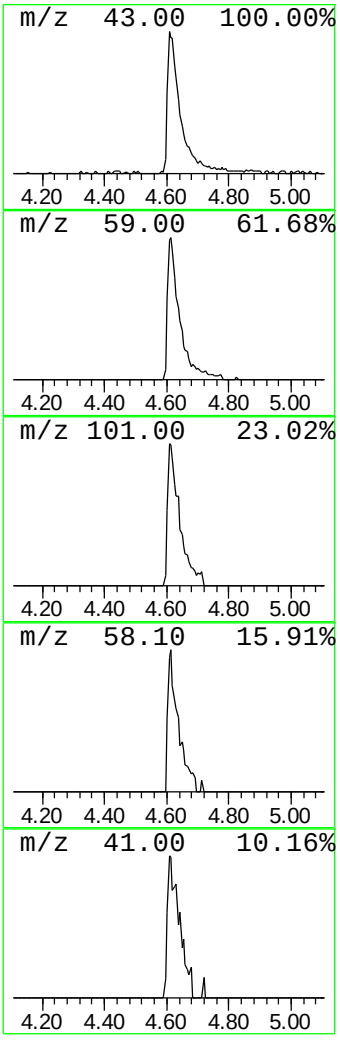
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	5.73 ng	145430	1,4-Dichlorobenzene-d4	7.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
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Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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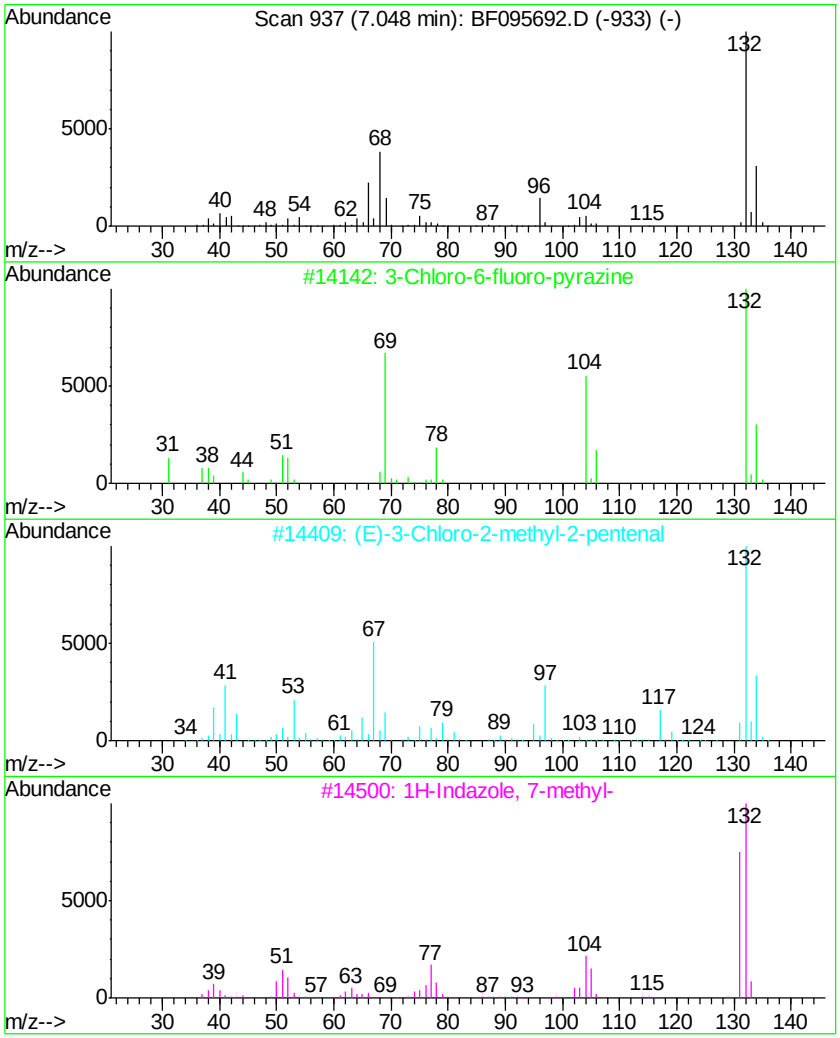
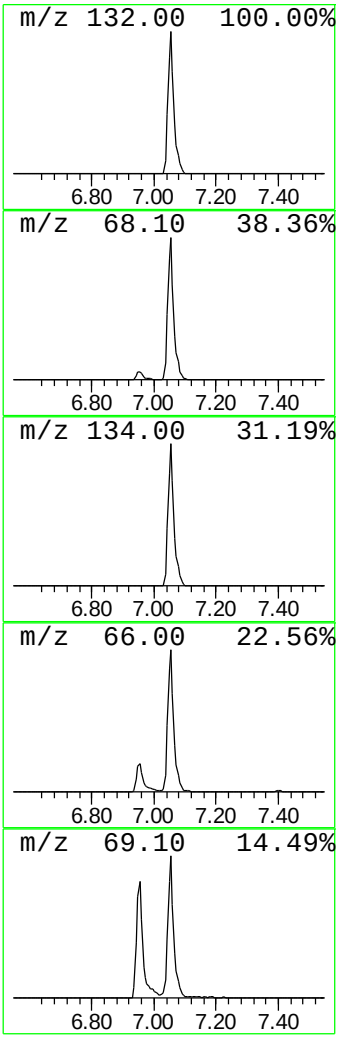
Peak Number 3 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	76.66 ng	1945570	1,4-Dichlorobenzene-d4	7.40

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	25
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
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Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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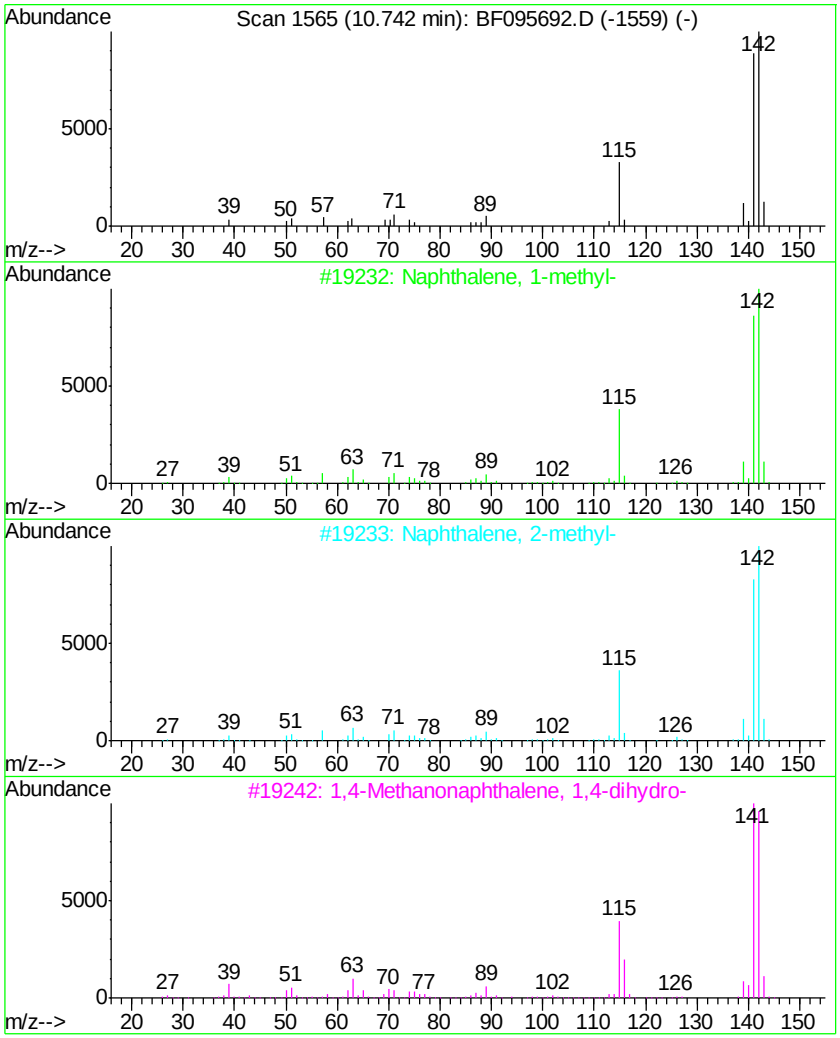
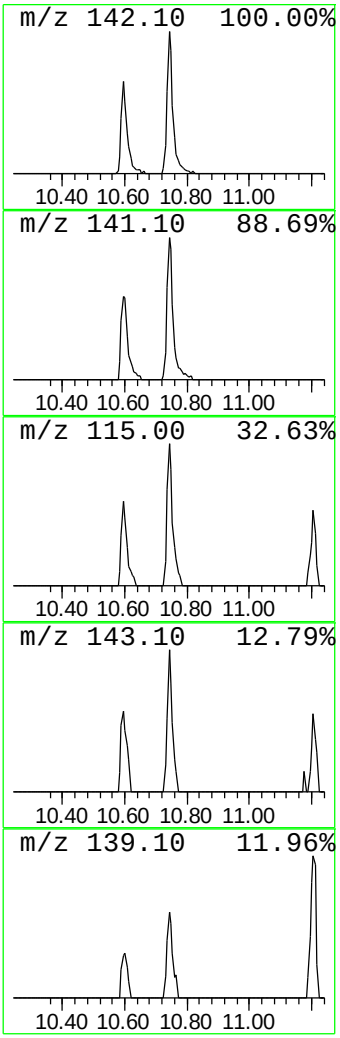
Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.09 ng	70292	Naphthalene-d8	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
5	Benzocycloheptatriene	142	C11H10	000264-09-5	90





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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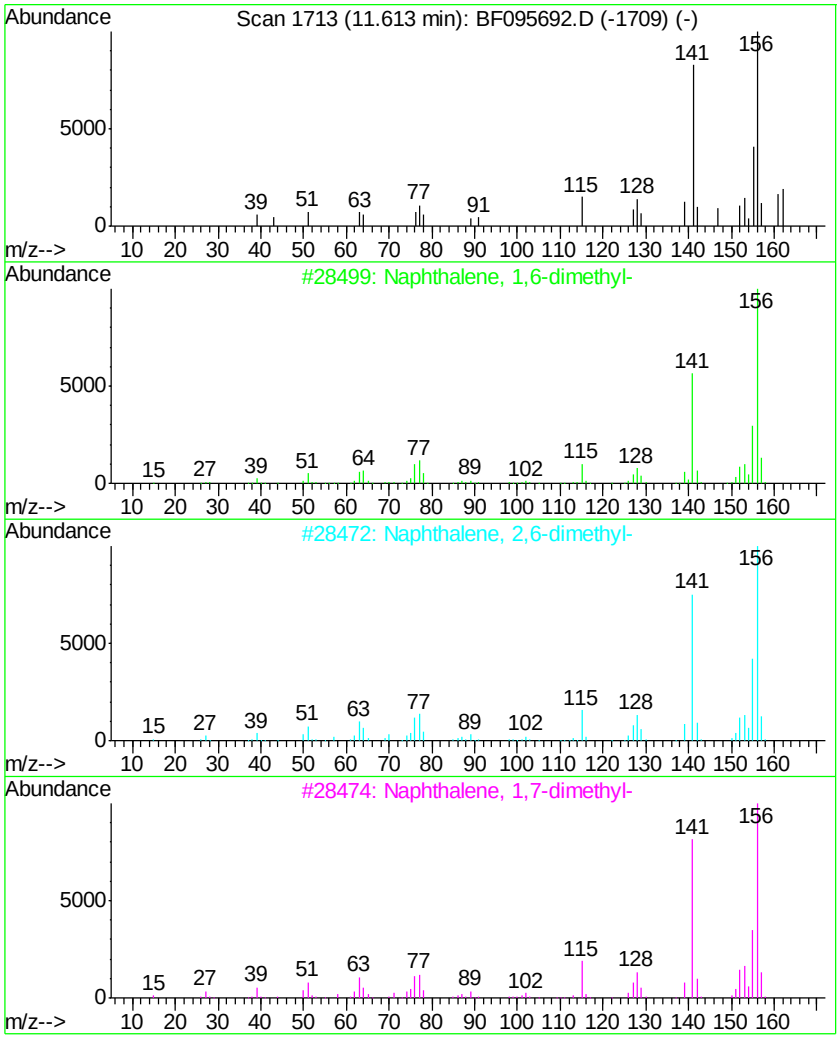
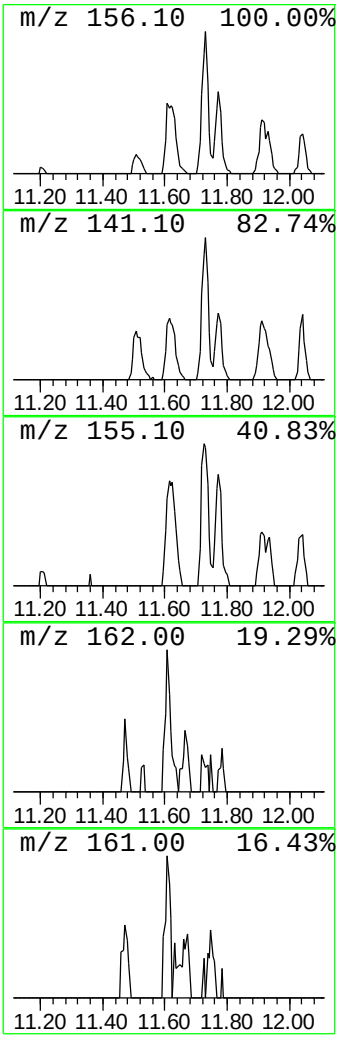
Peak Number 6 Naphthalene, 1,6-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	2.00 ng	67489	Acenaphthene-d10	12.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
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Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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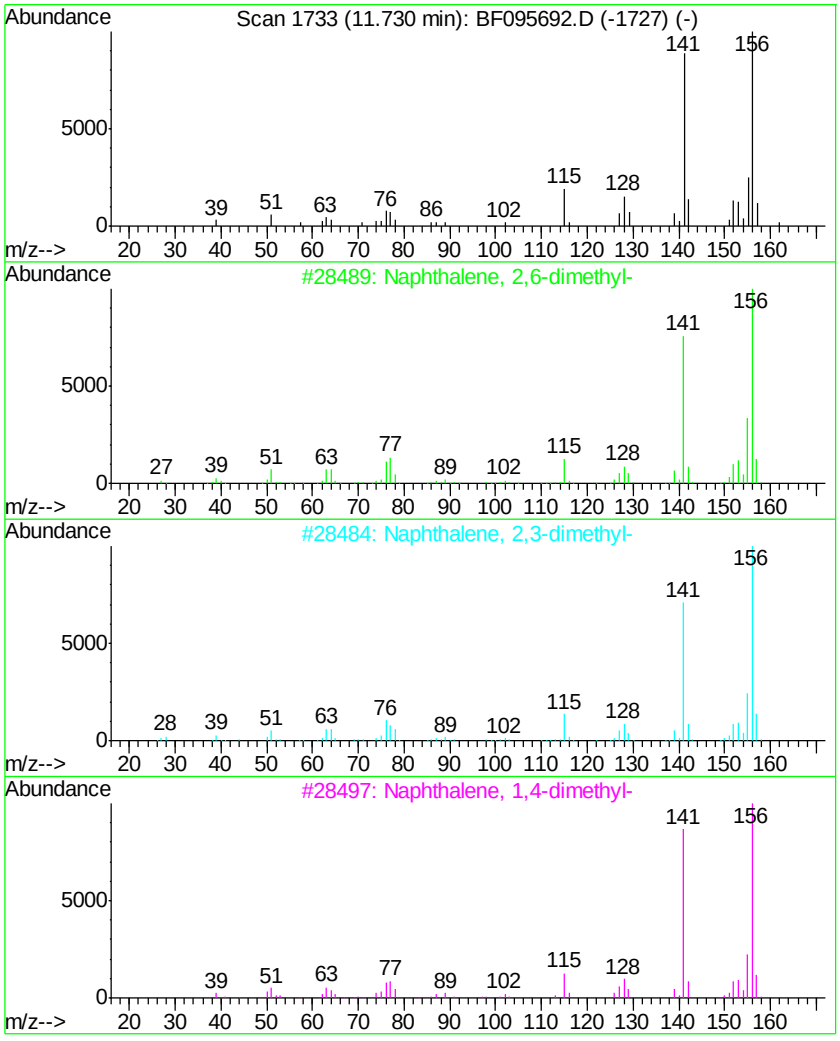
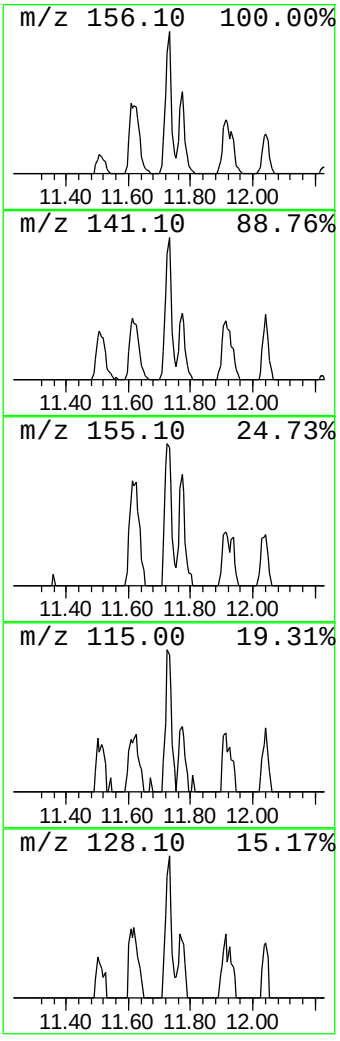
Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.47 ng	83329	Acenaphthene-d10	12.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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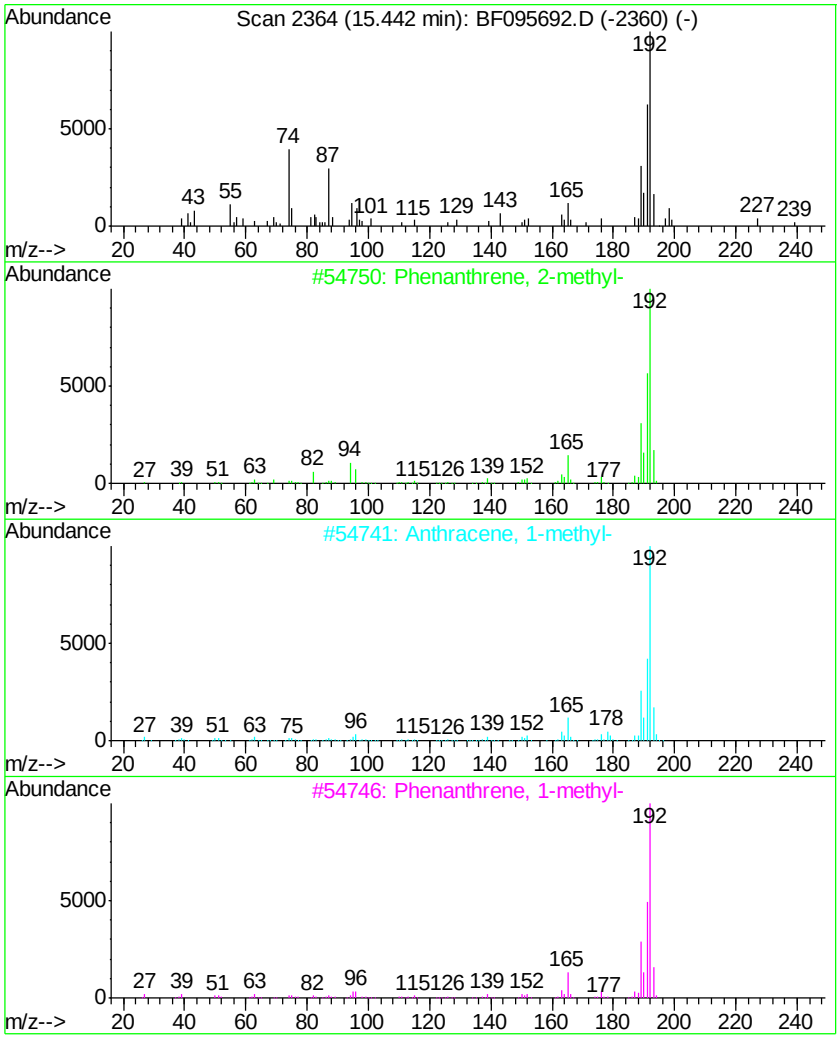
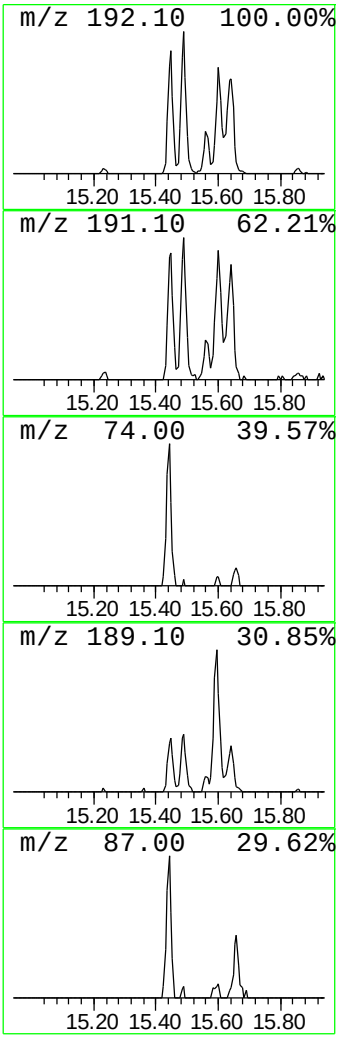
Peak Number 9 Phenanthrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	3.82 ng	110202	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095692.D
Acq On : 6 Jun 2017 1:22
Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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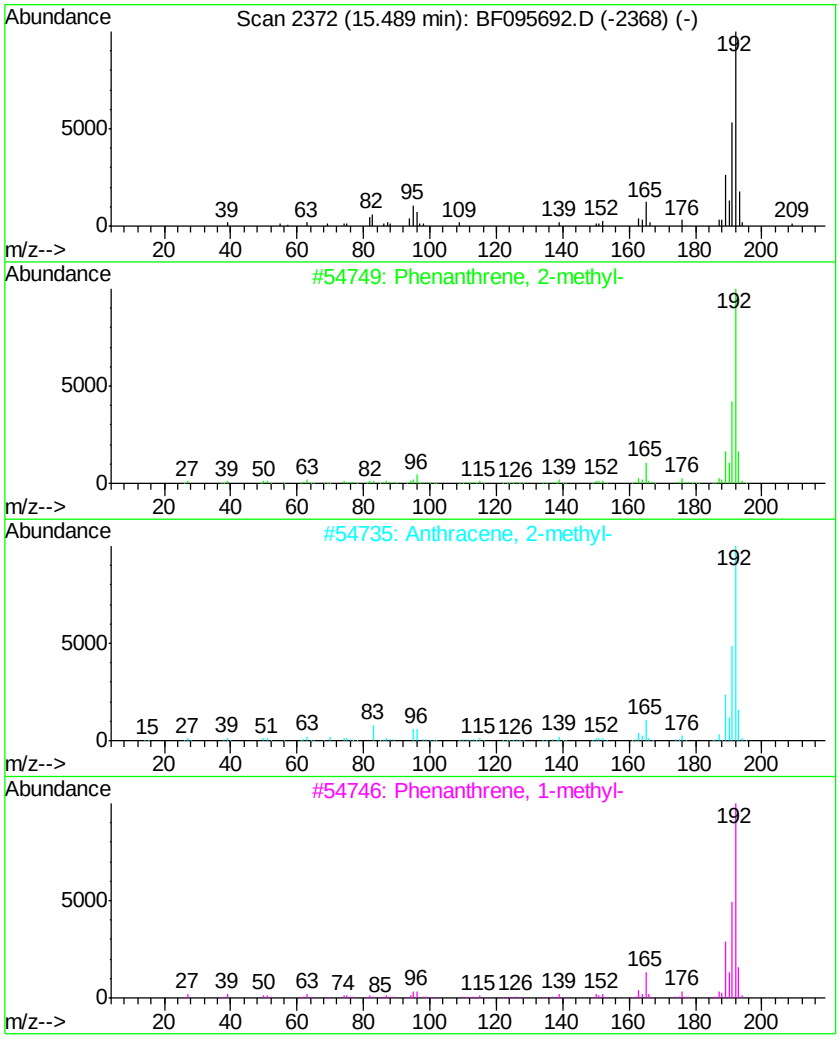
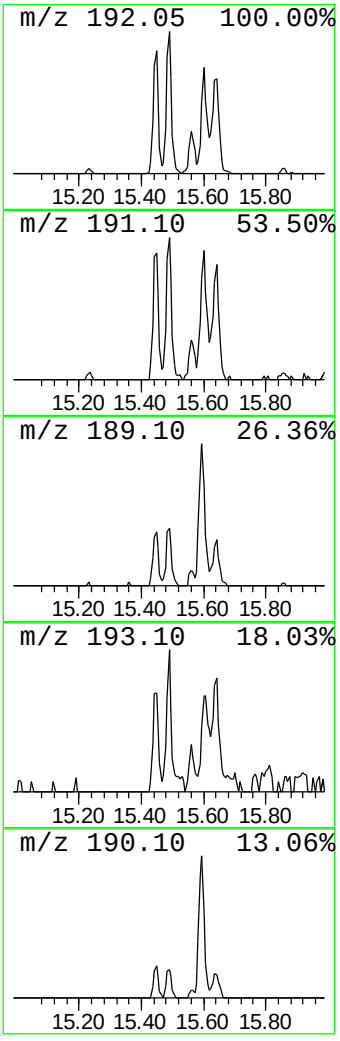
Peak Number 10 1H-Indene, 2-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	2.81 ng	80996	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95





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Data File : BF095692.D
Acq On : 6 Jun 2017 1:22
Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

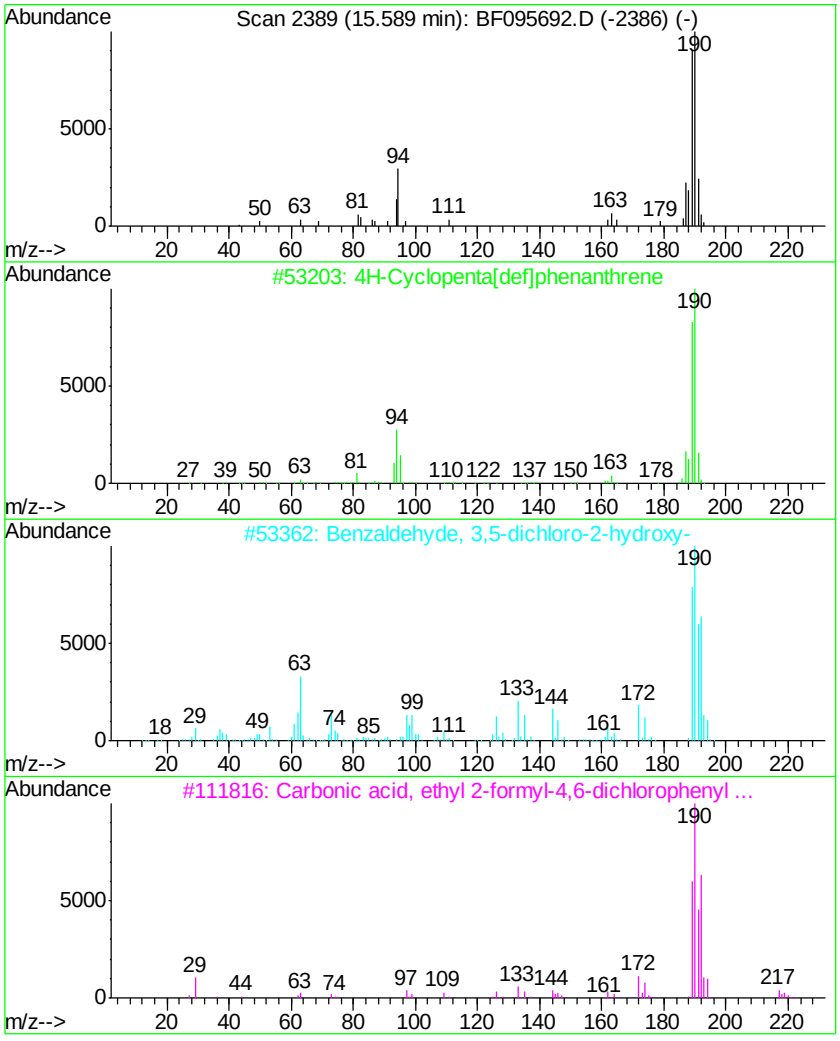
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

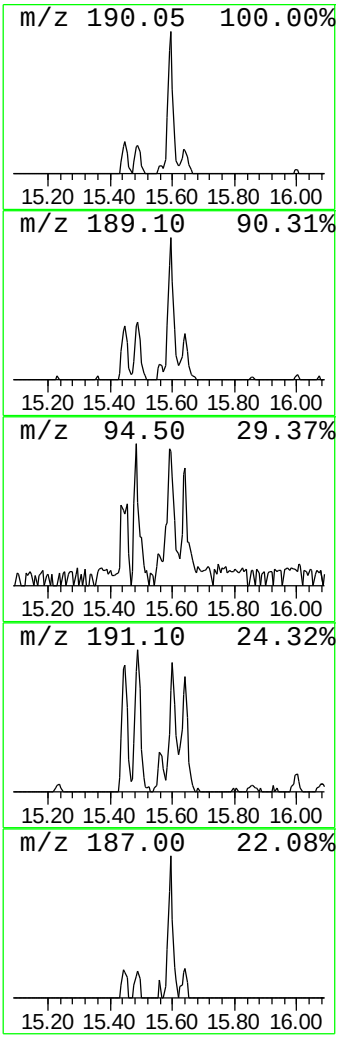
****

Peak Number 11 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	4.02 ng	116059	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	27
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	22





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

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

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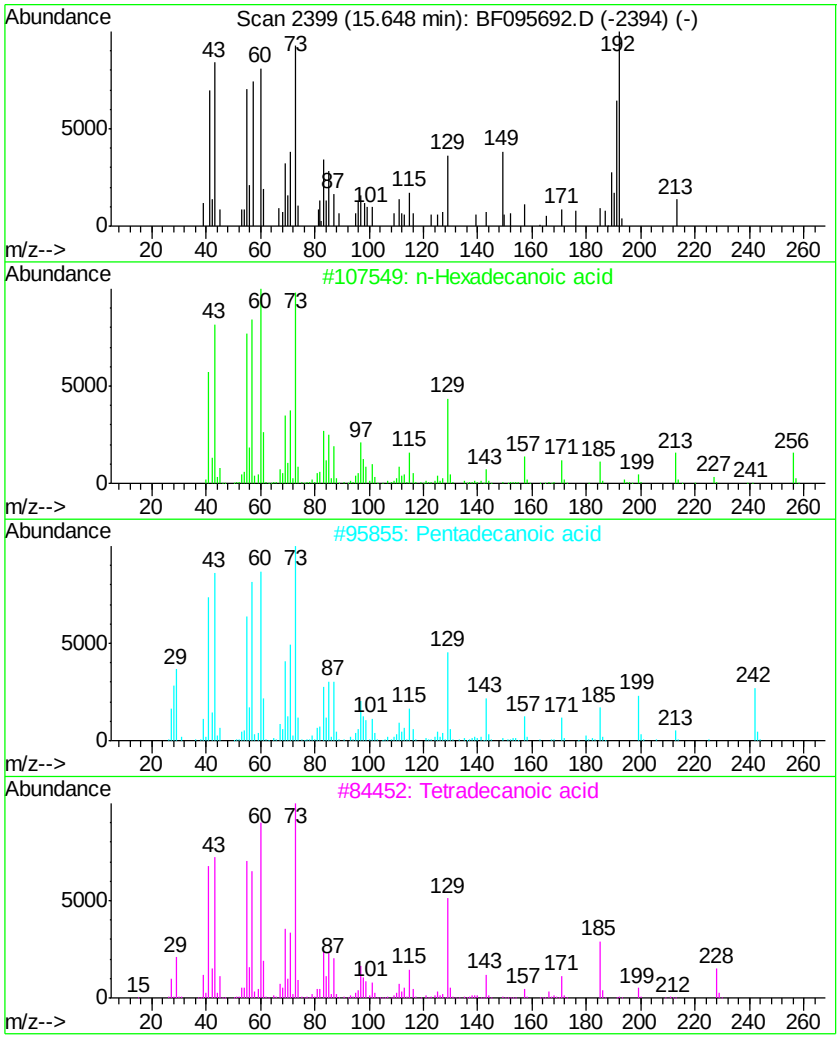
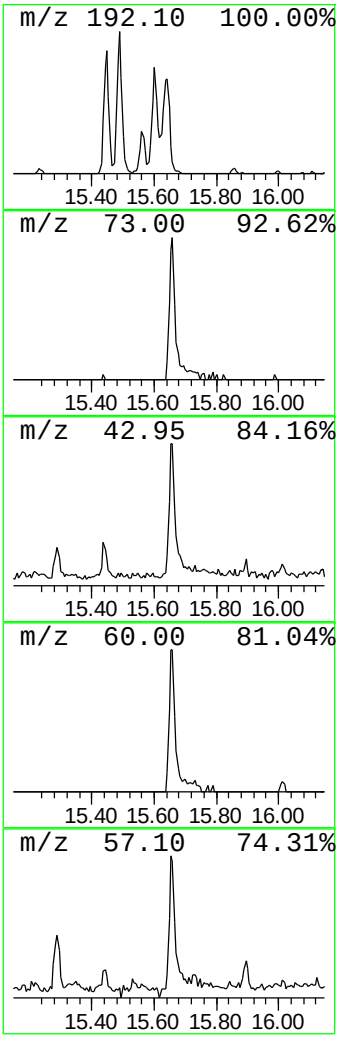
Peak Number 12 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	6.95 ng	200478	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	15





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Operator : SJ/MA
Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Integration Parameters: LSCINT.P

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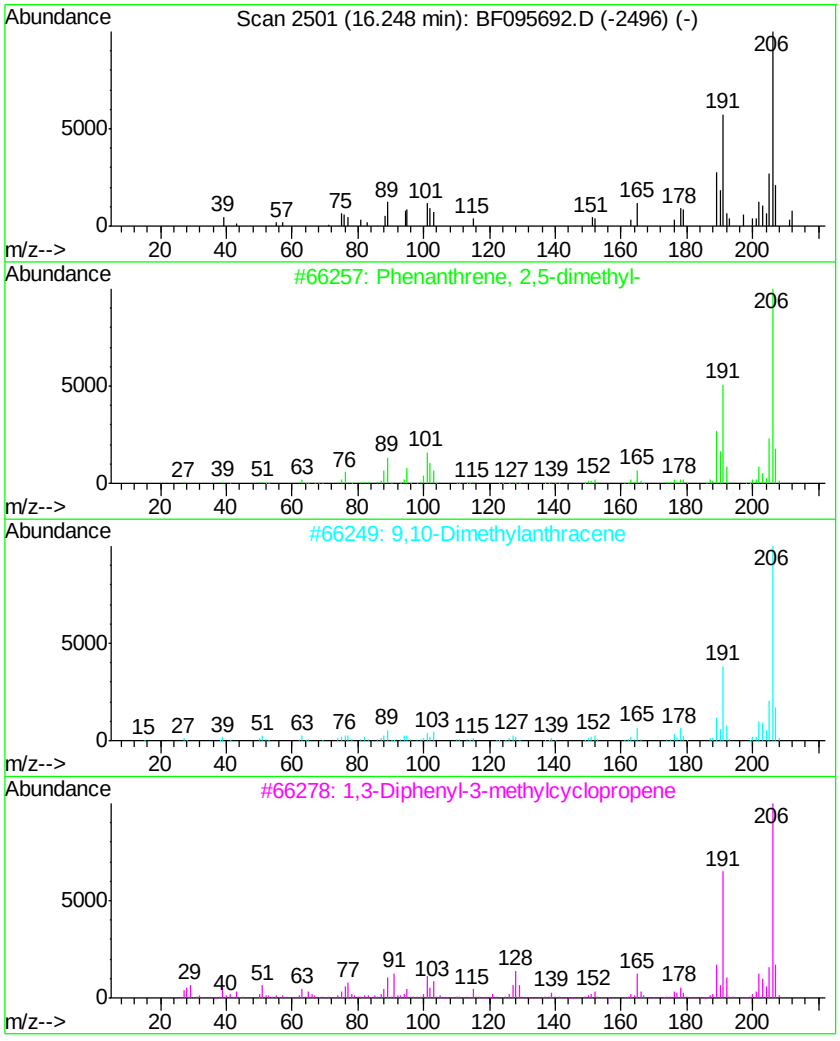
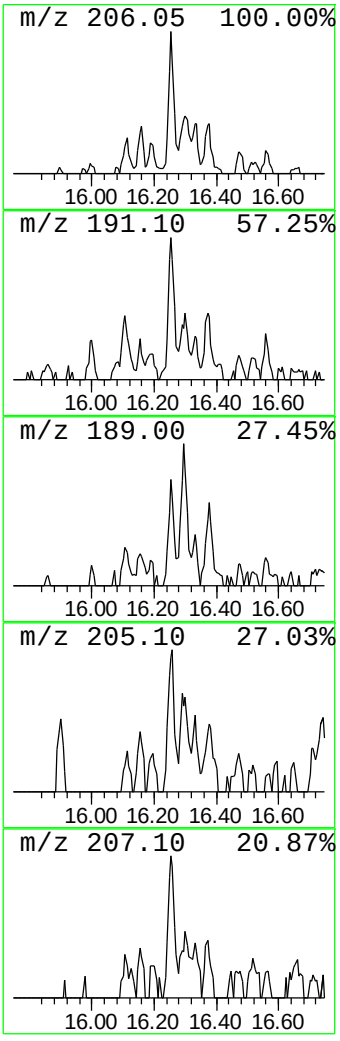
Peak Number 13 Phenanthrene, 2,5-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.35 ng	67772	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	94
3	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	94
4	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	93
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93





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Sample : I3466-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-4672-060217

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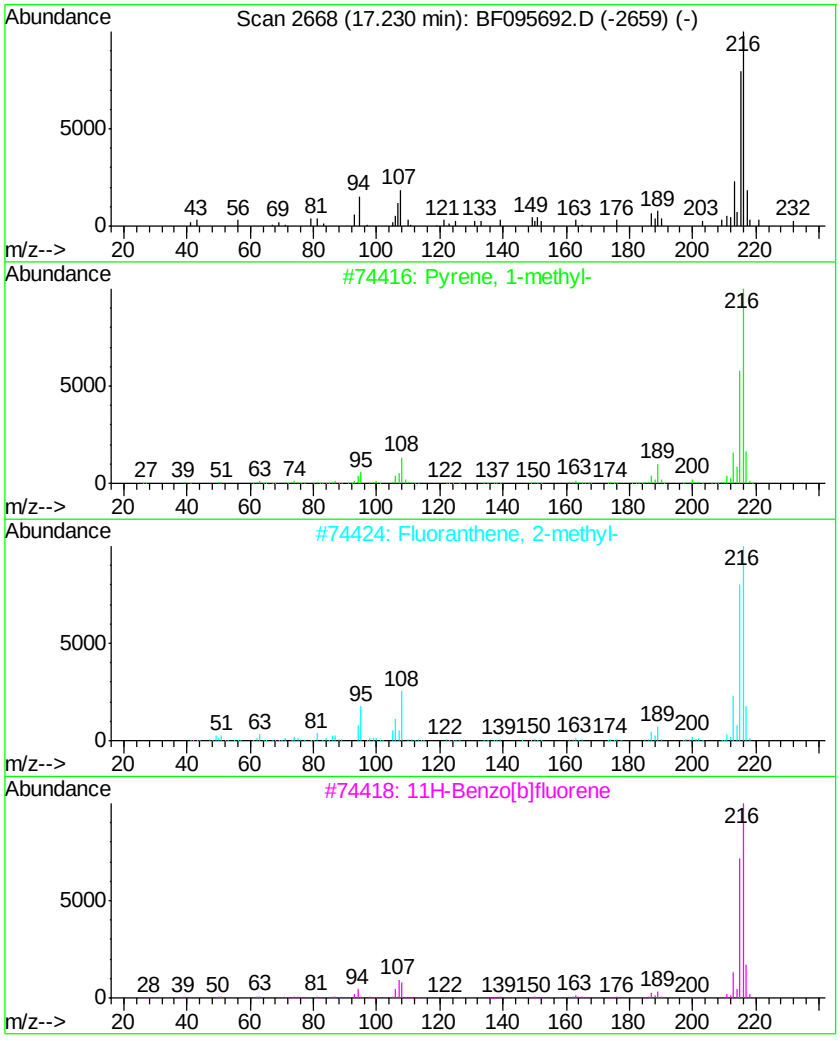
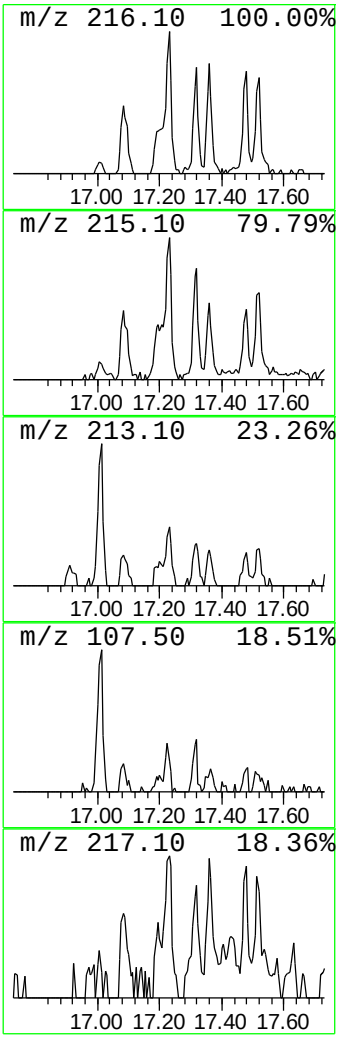
Peak Number 14 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	2.58 ng	89097	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





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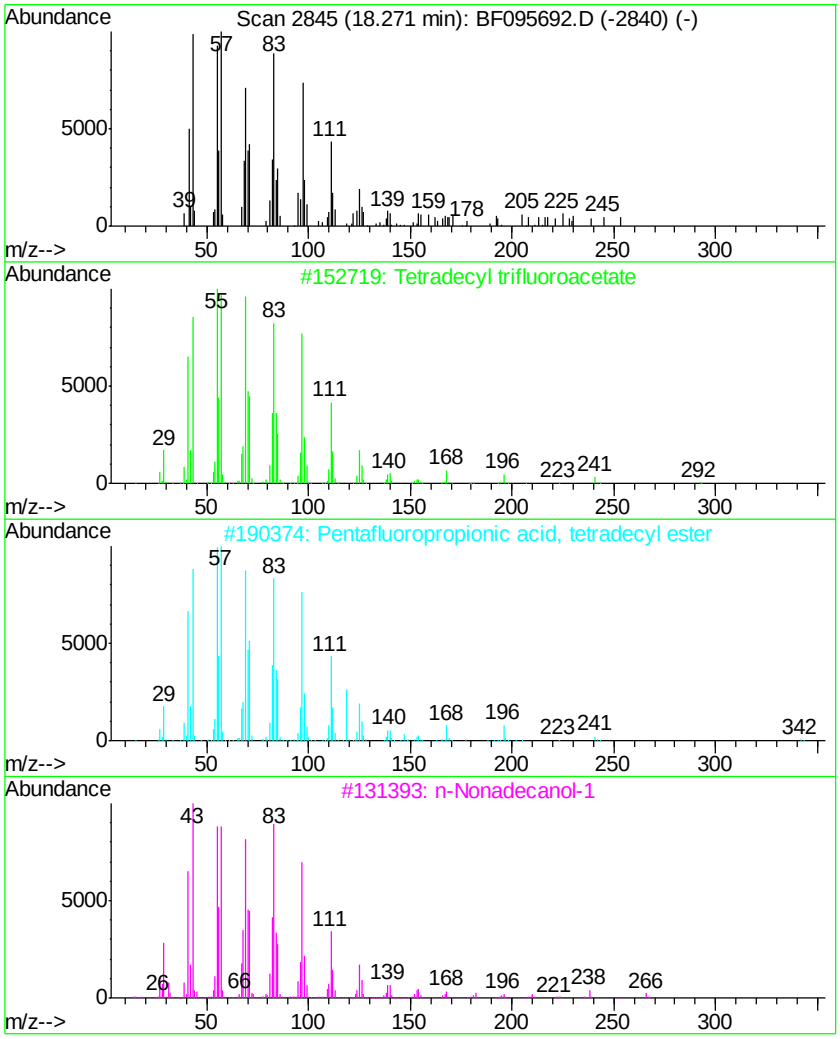
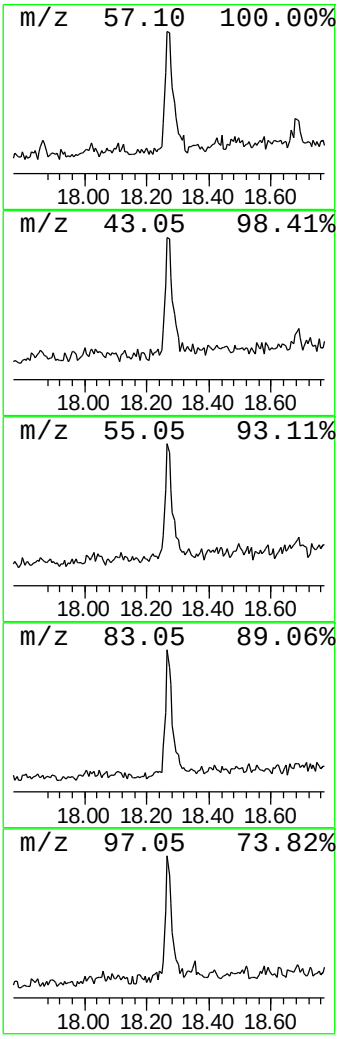
Peak Number 15 Tetradecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	4.96 ng	171523	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





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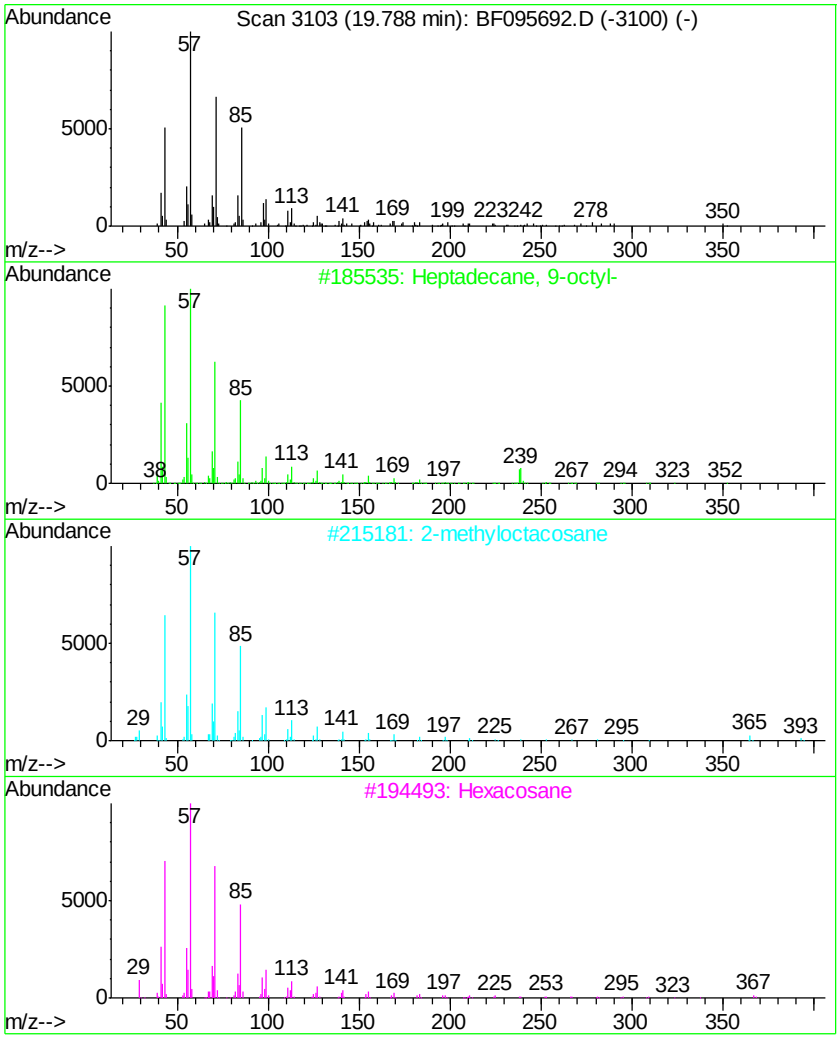
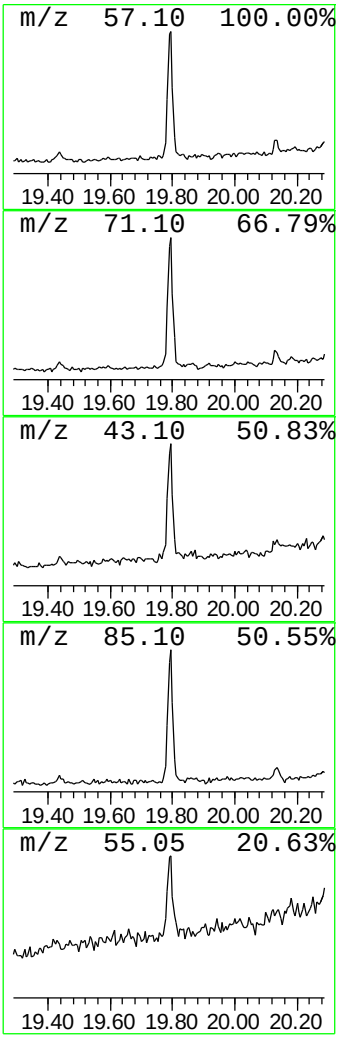
Peak Number 16 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	7.04 ng	161363	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Triacontane	422	C30H62	000638-68-6	86
5	Heneicosane	296	C21H44	000629-94-7	86





Tentatively Identified Compound (LSC) summary

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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...	4.61	5.7	ng	145430	1	7.40	507615	20.0
unknown7.05	7.05	76.7	ng	1945570	1	7.40	507615	20.0
Naphthalene, 1-me...	10.74	2.1	ng	70292	2	9.43	672148	20.0
Naphthalene, 1,6-...	11.61	2.0	ng	67489	3	12.25	674560	20.0
Naphthalene, 2,6-...	11.73	2.5	ng	83329	3	12.25	674560	20.0
Phenanthrene, 2-m...	15.44	3.8	ng	110202	4	14.64	577305	20.0
1H-Indene, 2-phenyl-	15.49	2.8	ng	80996	4	14.64	577305	20.0
4H-Cyclopenta[def...	15.59	4.0	ng	116059	4	14.64	577305	20.0
n-Hexadecanoic acid	15.65	7.0	ng	200478	4	14.64	577305	20.0
Phenanthrene, 2,5...	16.25	2.4	ng	67772	4	14.64	577305	20.0
Pyrene, 1-methyl-	17.23	2.6	ng	89097	5	18.35	691888	20.0
Tetradecyl triflu...	18.27	5.0	ng	171523	5	18.35	691888	20.0
Heptadecane, 9-oc...	19.79	7.0	ng	161363	6	20.02	458125	20.0