LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM052419\
Data File : BM020562.D
Acq On : 25 May 2019 03:56
Operator : JU/SJ
Sample : K2647-11 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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	5.240	378	383	399	rBV	418283	791811	26.79%	2.748%
2	6.840	648	655	673	rBV	391317	883644	29.90%	3.066%
3	7.187	708	714	729	rBV	480958	921800	31.19%	3.199%
4	7.657	788	794	808	rBV	223332	421609	14.27%	1.463%
5	7.975	841	848	865	rBV	407030	739722	25.03%	2.567%
6	8.834	987	994	1016	rBV	209658	521581	17.65%	1.810%
7	10.445	1262	1268	1279	rBV	296310	549752	18.60%	1.908%
8	12.927	1683	1690	1710	rBV	955173	1532463	51.85%	5.318%
9	13.774	1826	1834	1841	rBV	95966	158898	5.38%	0.551%
10	14.039	1873	1879	1889	rBV	55683	99877	3.38%	0.347%
11	14.316	1919	1926	1934	rBV2	601237	950879	32.17%	3.300%
12	14.374	1934	1936	1944	rVB2	21961	37078	1.25%	0.129%
13	14.710	1987	1993	1998	rBV5	18065	34237	1.16%	0.119%
14	14.927	2025	2030	2036	rBV5	16541	31452	1.06%	0.109%
15	15.151	2062	2068	2072	rVV3	24525	34213	1.16%	0.119%
16	15.368	2098	2105	2109	rBV3	25072	47106	1.59%	0.163%
17	15.557	2129	2137	2139	rBV6	11807	30526	1.03%	0.106%
18	15.815	2175	2181	2199	rVB	939353	1527917	51.70%	5.302%
19	16.015	2211	2215	2216	rBV2	44255	52297	1.77%	0.181%
20	16.380	2269	2277	2280	rBV5	20315	50671	1.71%	0.176%
21	16.804	2345	2349	2354	rBV2	45749	66327	2.24%	0.230%
22	16.857	2354	2358	2360	rVV4	29562	43214	1.46%	0.150%
23	16.892	2361	2364	2371	rVB3	25489	43653	1.48%	0.151%
24	17.068	2387	2394	2398	rBV2	898964	1342595	45.43%	4.659%
25	17.109	2398	2401	2410	rVV	377657	568791	19.25%	1.974%
26	17.204	2412	2417	2426	rBV	94747	177571	6.01%	0.616%
27	17.545	2471	2475	2478	rVB2	46964	54284	1.84%	0.188%
28	17.651	2489	2493	2497	rVB3	22998	36997	1.25%	0.128%
29	17.727	2501	2506	2513	rBV	368599	455035	15.40%	1.579%
30	17.945	2538	2543	2547	rBV	122665	221922	7.51%	0.770%
31	17.992	2547	2551	2557	rVV	135819	219334	7.42%	0.761%
32	18.074	2561	2565	2570	rVV2	50752	87520	2.96%	0.304%
33	18.139	2570	2576	2579	rVV2	152044	293605	9.93%	1.019%
34	18.174	2580	2582	2589	rVB	82106	104445	3.53%	0.362%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM052419\
Data File : BM020562.D
Acq On : 25 May 2019 03:56
Operator : JU/SJ
Sample : K2647-11 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.239	2589	2593	2598	rBV3	44598	68175	2.31%	0.237%
36	18.445	2624	2628	2634	rBV	44495	80387	2.72%	0.279%
37	18.503	2634	2638	2646	rVB3	47692	80437	2.72%	0.279%
38	18.692	2667	2670	2675	rVB2	31505	42184	1.43%	0.146%
39	18.745	2675	2679	2682	rBV	51548	70885	2.40%	0.246%
40	18.786	2682	2686	2689	rVB2	37196	45909	1.55%	0.159%
41	18.874	2694	2701	2704	rBV2	1199811	1621697	54.87%	5.627%
42	18.909	2704	2707	2719	rVB2	1474630	2086025	70.58%	7.239%
43	19.039	2719	2729	2736	rBV5	213280	437649	14.81%	1.519%
44	19.133	2740	2745	2751	rBV	1030327	1403045	47.47%	4.869%
45	19.462	2797	2801	2803	rBV2	169634	240828	8.15%	0.836%
46	19.498	2803	2807	2815	rVV	967459	1431488	48.44%	4.967%
47	19.568	2815	2819	2824	rVV	90498	133763	4.53%	0.464%
48	19.698	2836	2841	2852	rBV	2295155	2955363	100.00%	10.255%
49	19.827	2857	2863	2871	rBV4	83867	259036	8.76%	0.899%
50	19.992	2889	2891	2896	rVB	194717	232238	7.86%	0.806%
51	20.092	2905	2908	2912	rBV	128547	156769	5.30%	0.544%
52	20.150	2914	2918	2922	rVV2	130960	204058	6.90%	0.708%
53	20.292	2939	2942	2946	rBV	99790	138463	4.69%	0.480%
54	21.262	3100	3107	3110	rBV2	1215005	2252722	76.22%	7.817%
55	21.297	3110	3113	3120	rVB	520998	684059	23.15%	2.374%
56	23.503	3483	3488	3493	rBV2	592432	1060099	35.87%	3.679%

Sum of corrected areas: 28818105

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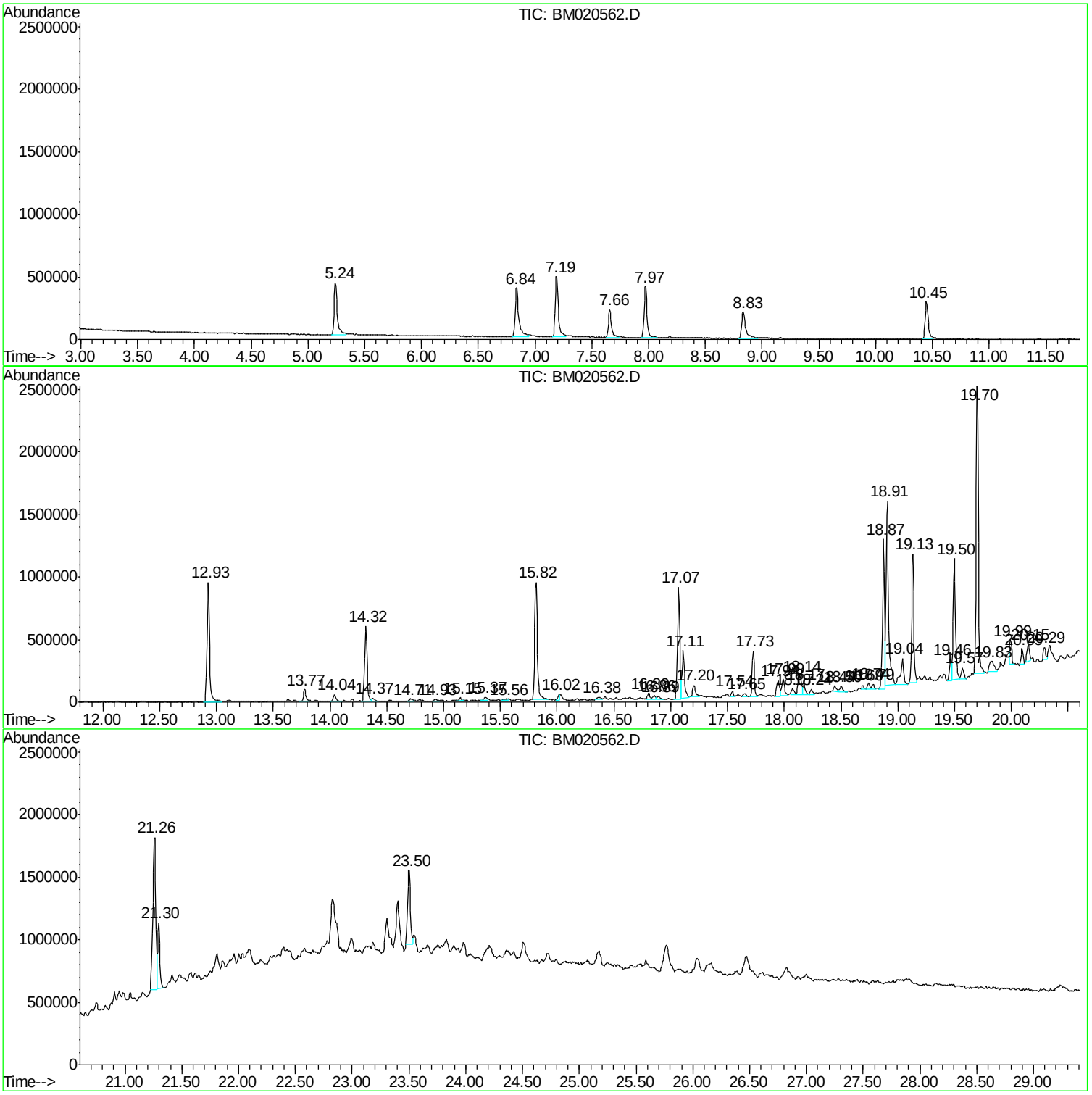
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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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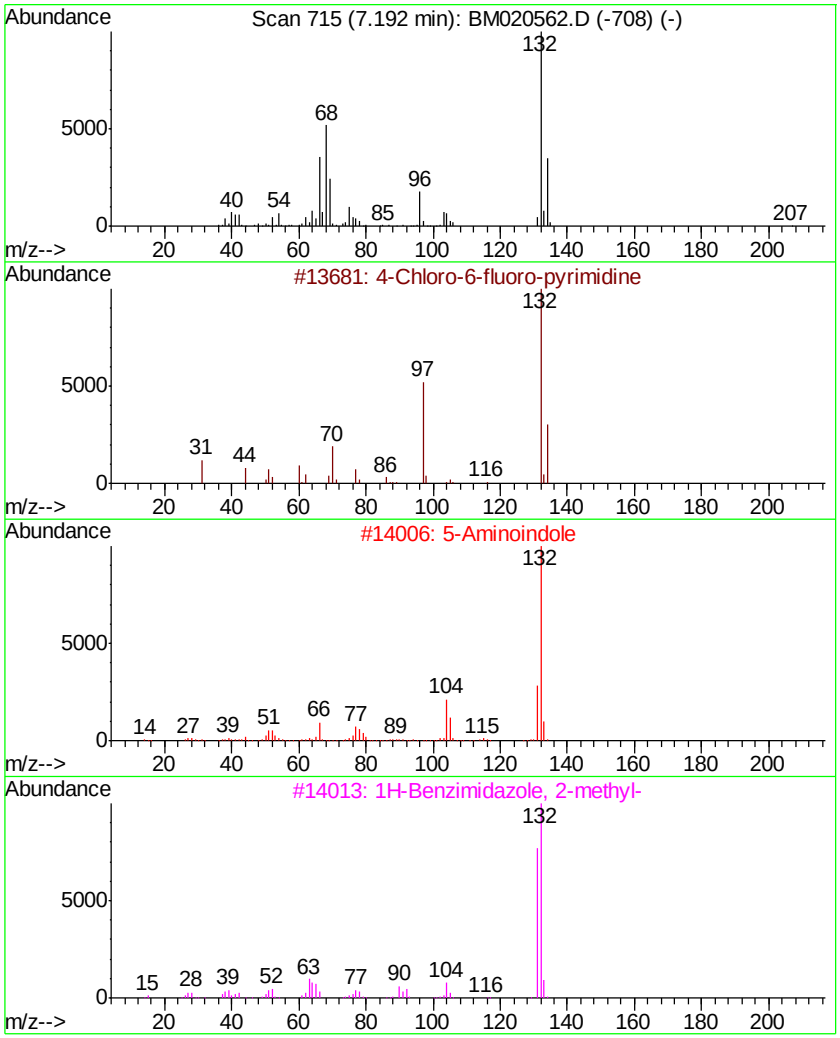
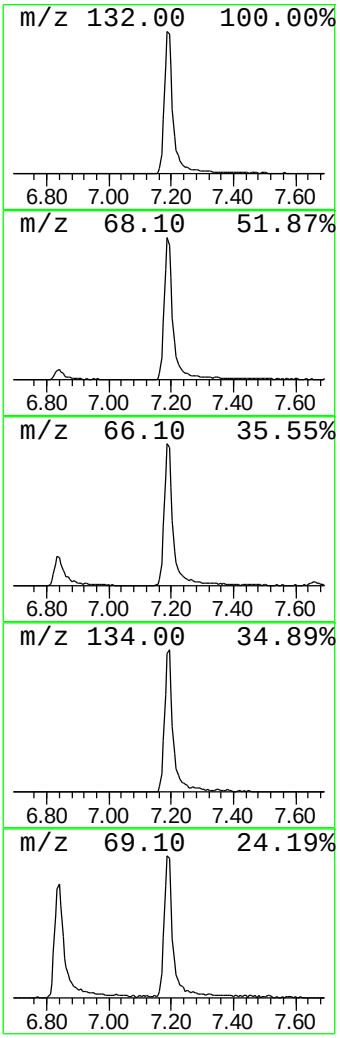
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	43.73 ng	921800	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16





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Operator : JU/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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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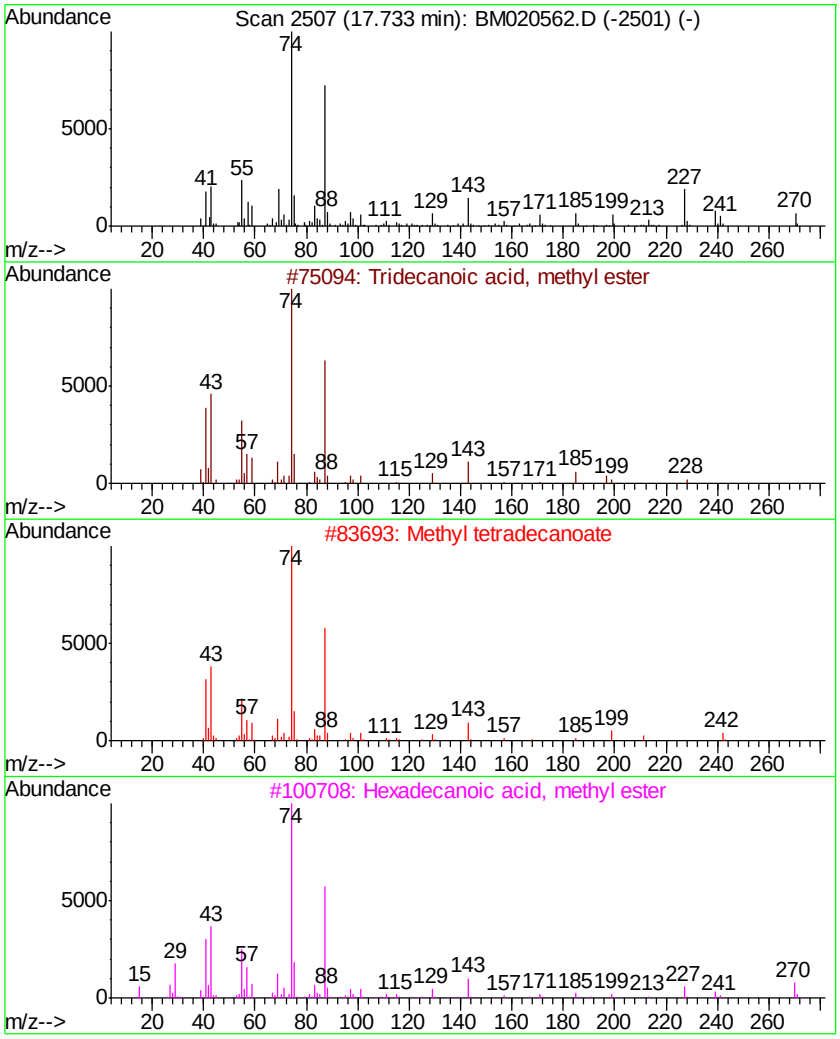
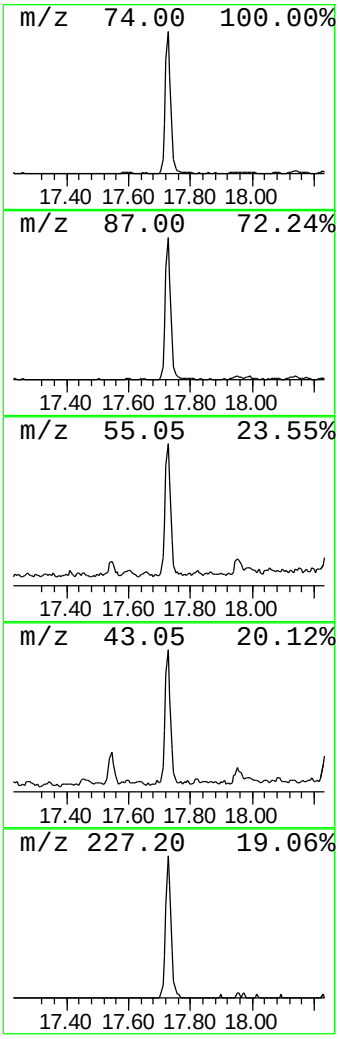
Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	6.78 ng	455035	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
5	9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	91





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Acq On : 25 May 2019 03:56
Operator : JU/SJ
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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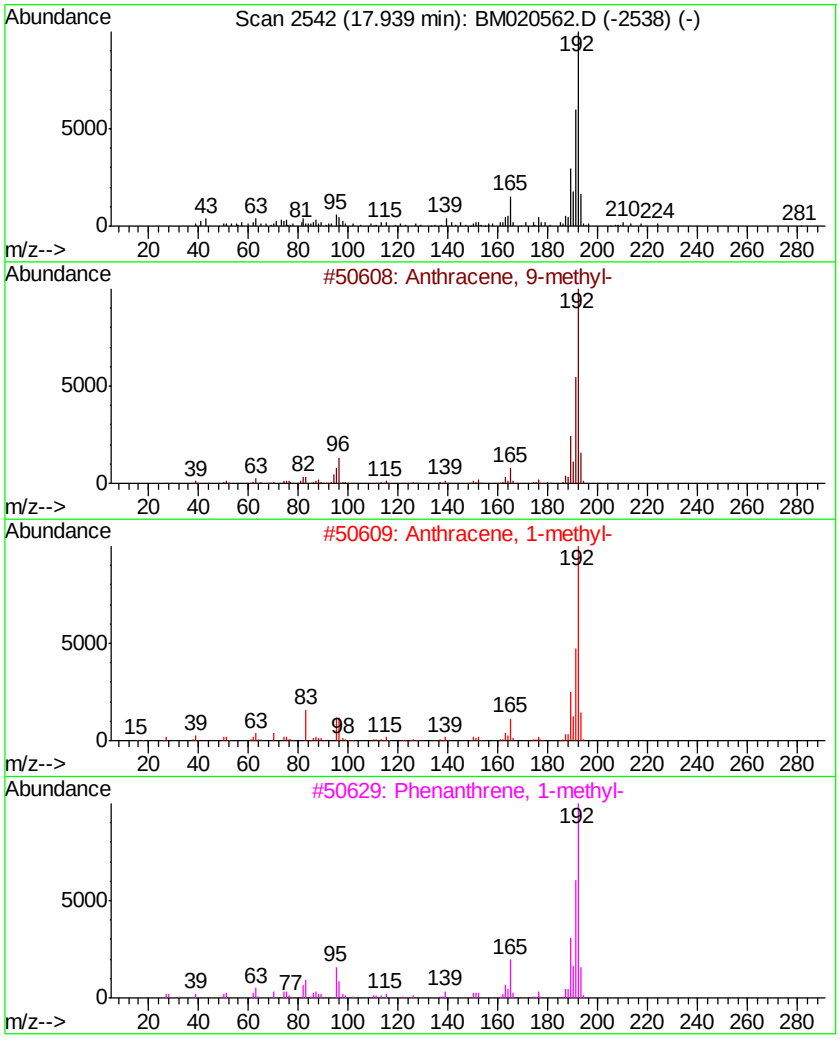
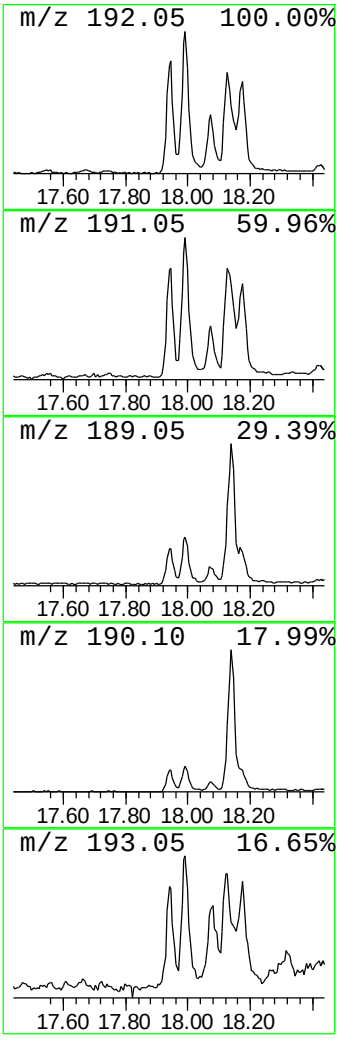
****

Peak Number 4 Anthracene, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	3.31 ng	221922	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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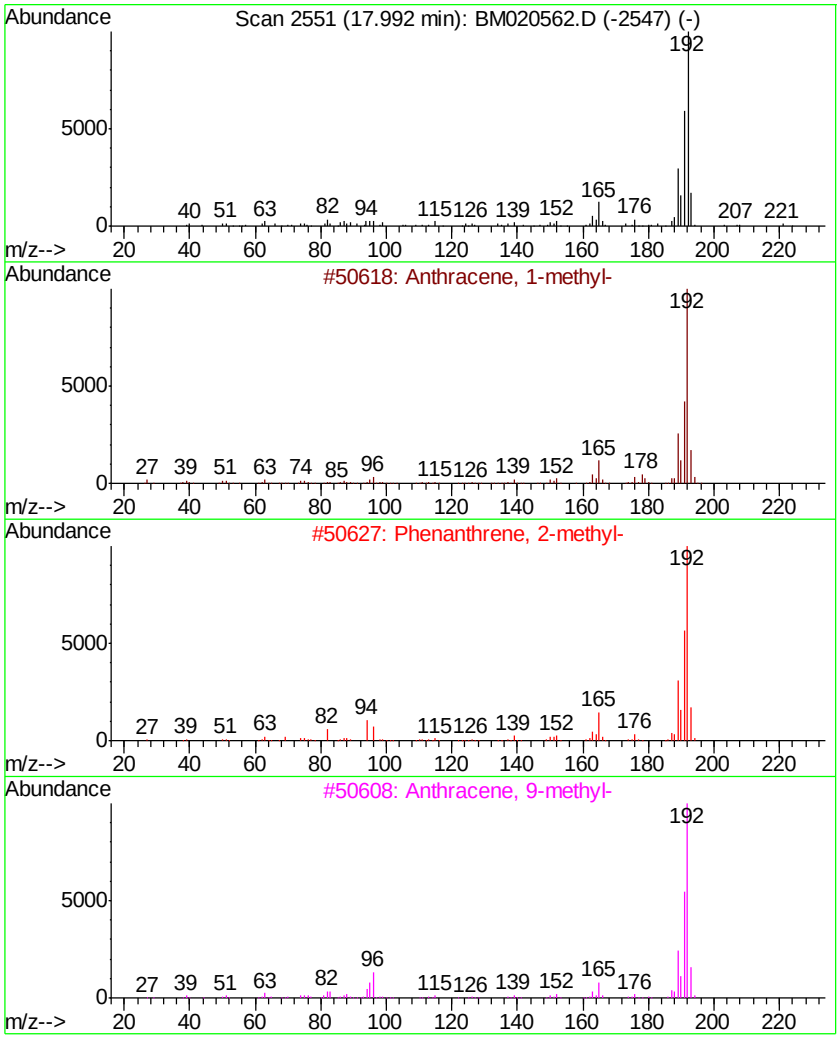
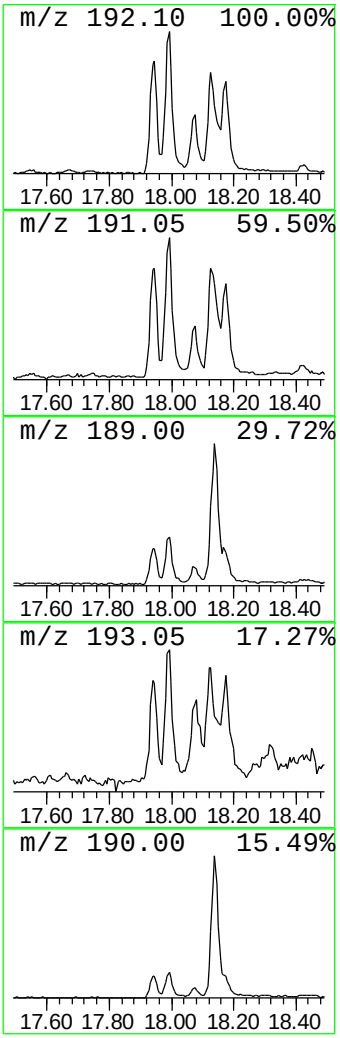
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	3.27 ng	219334	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	83





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Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

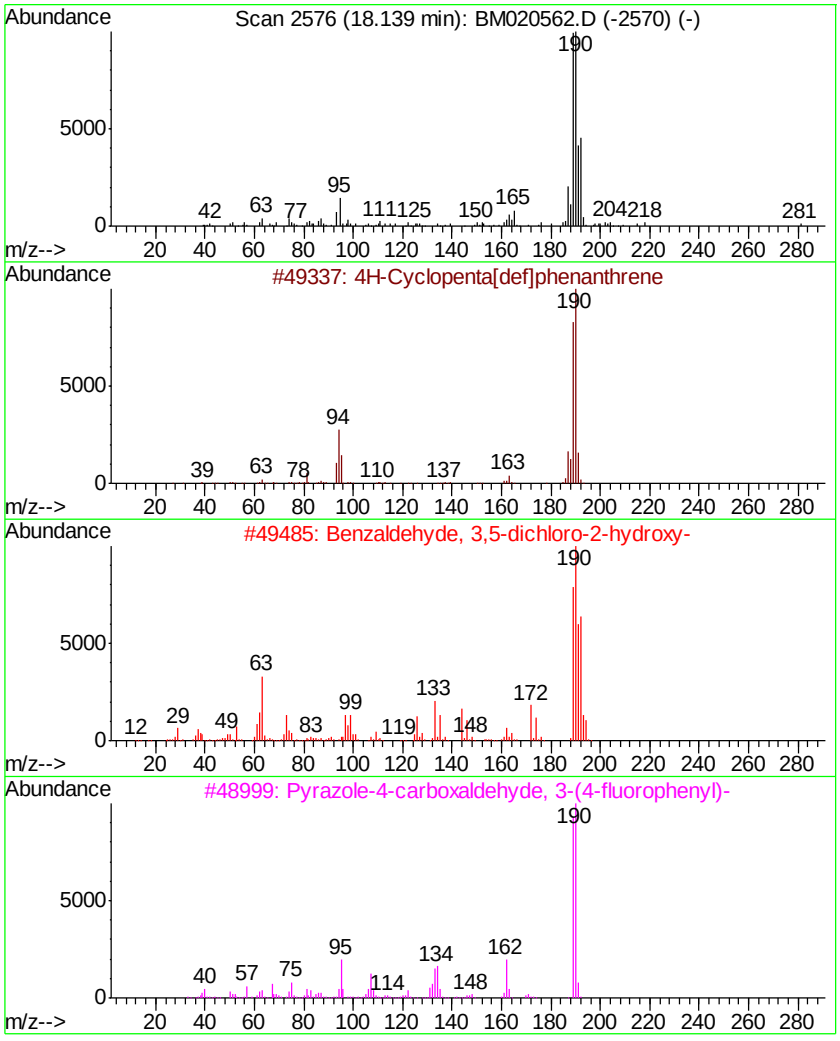
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

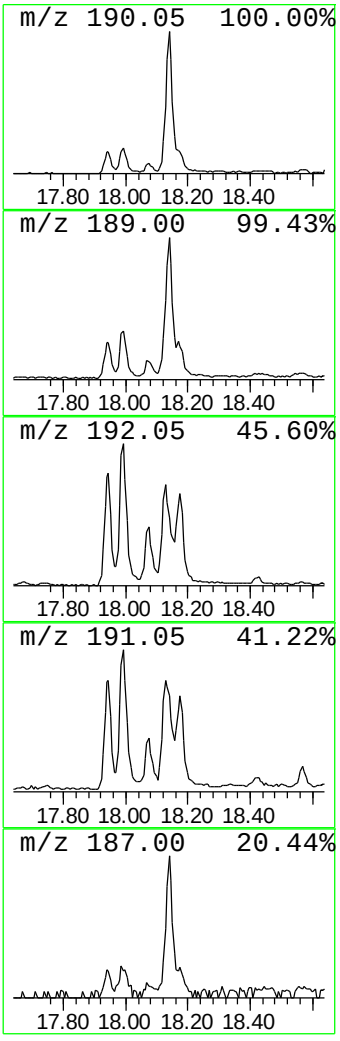
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	4.37 ng	293605	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	35





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

TIC Library : C:\DATABASE\NIST02.L
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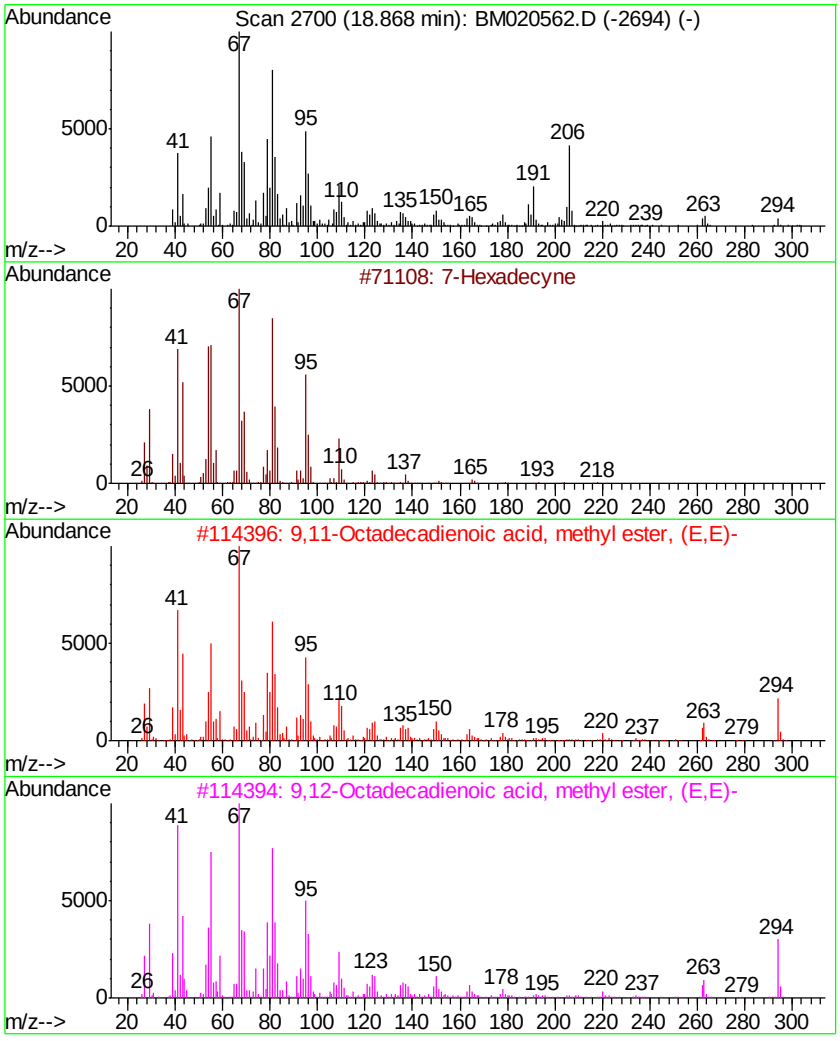
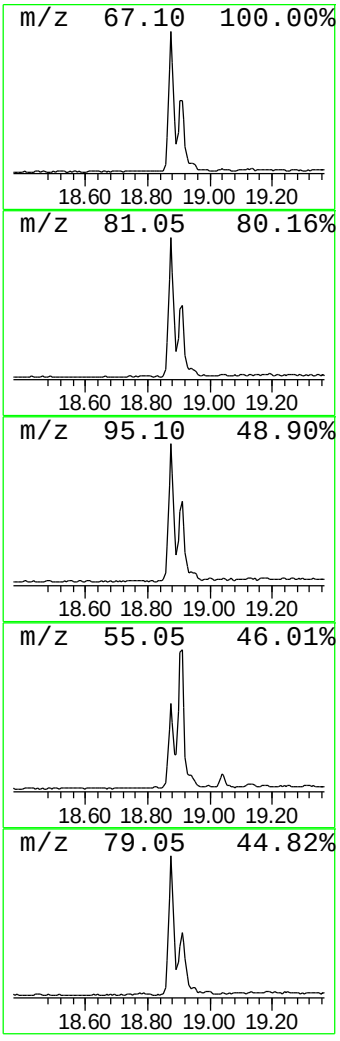
Peak Number 7 7-Hexadecyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.87	24.16 ng	1621700	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecyne	222	C16H30	074685-28-2	93
2	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	92
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	87
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	87
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	87





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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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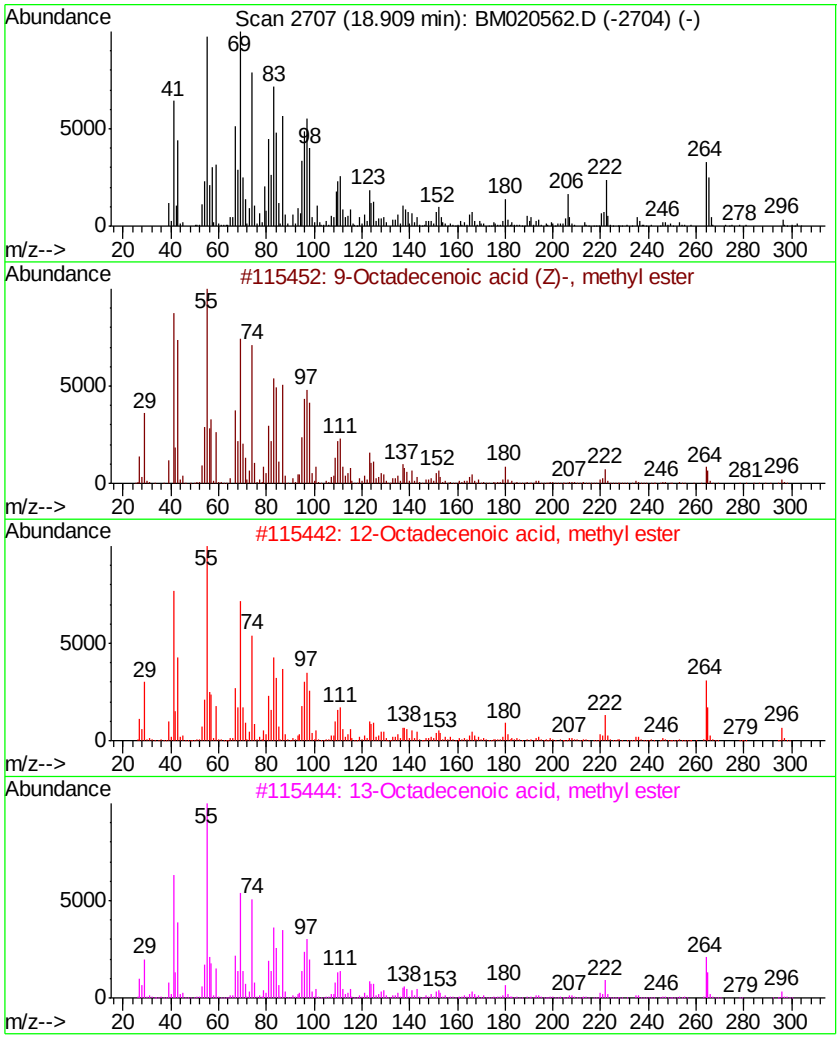
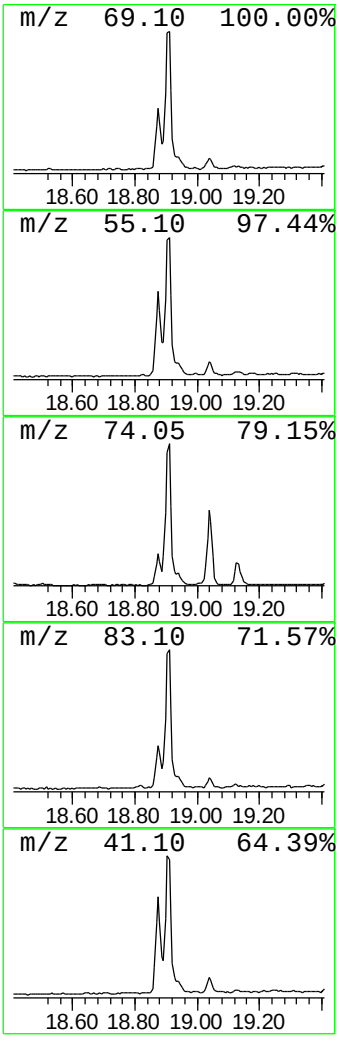
Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.91	31.07 ng	2086030	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99





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TIC Integration Parameters: LSCINT.P

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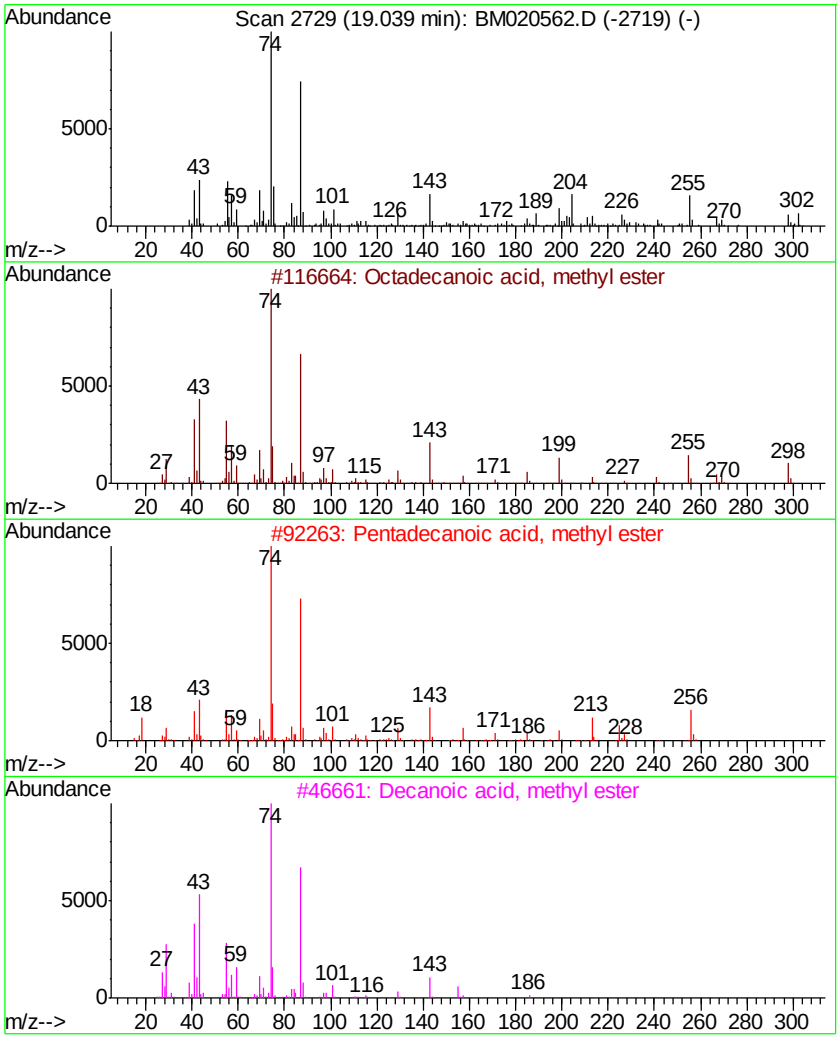
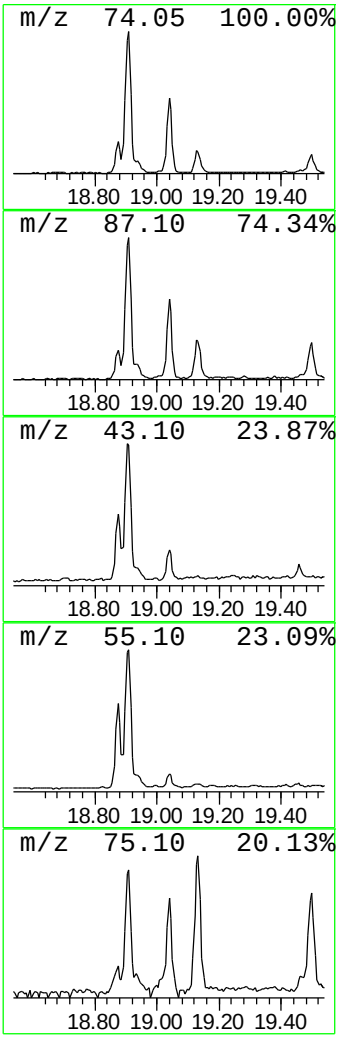
Peak Number 9 Octadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	6.52 ng	437649	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	98
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80





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Data File : BM020562.D
Acq On : 25 May 2019 03:56
Operator : JU/SJ
Sample : K2647-11 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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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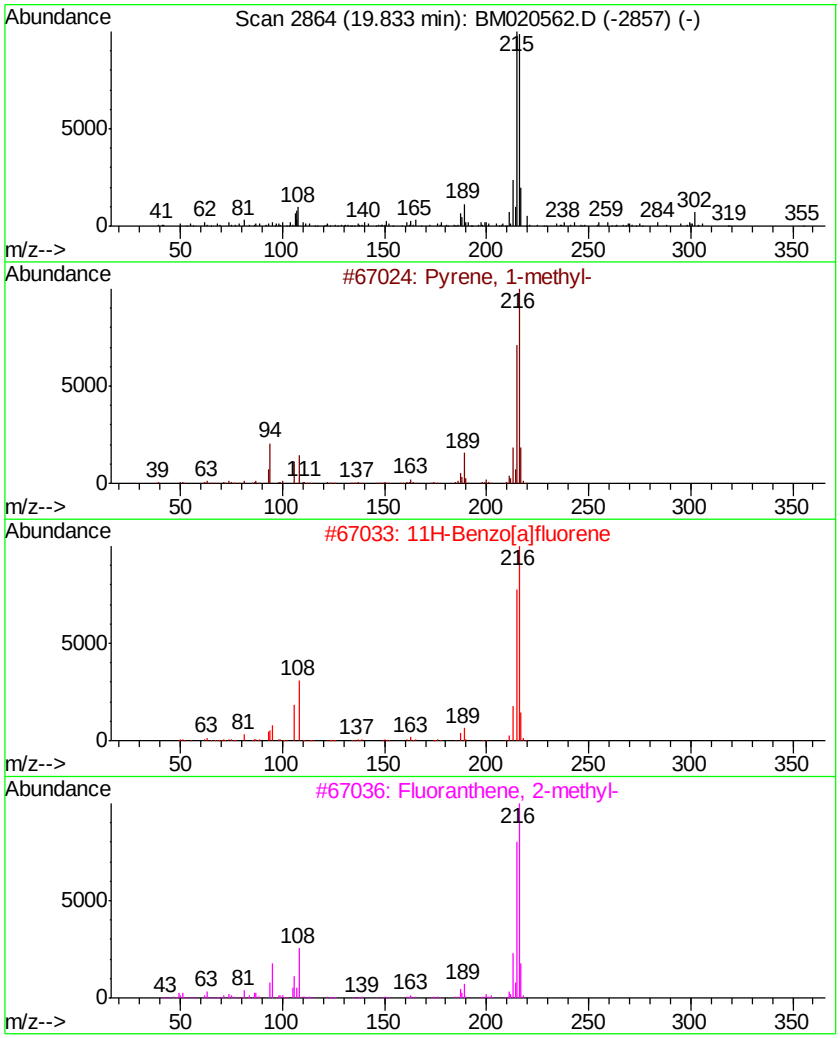
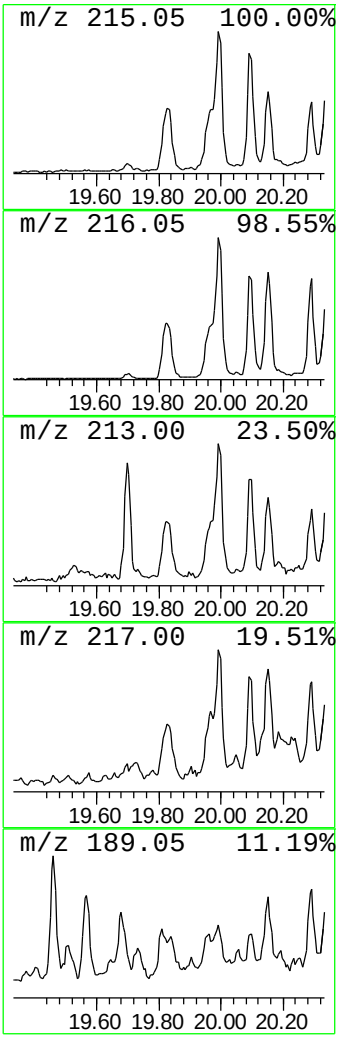
Peak Number 10 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.83	2.30 ng	259036	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM052419\
Data File : BM020562.D
Acq On : 25 May 2019 03:56
Operator : JU/SJ
Sample : K2647-11 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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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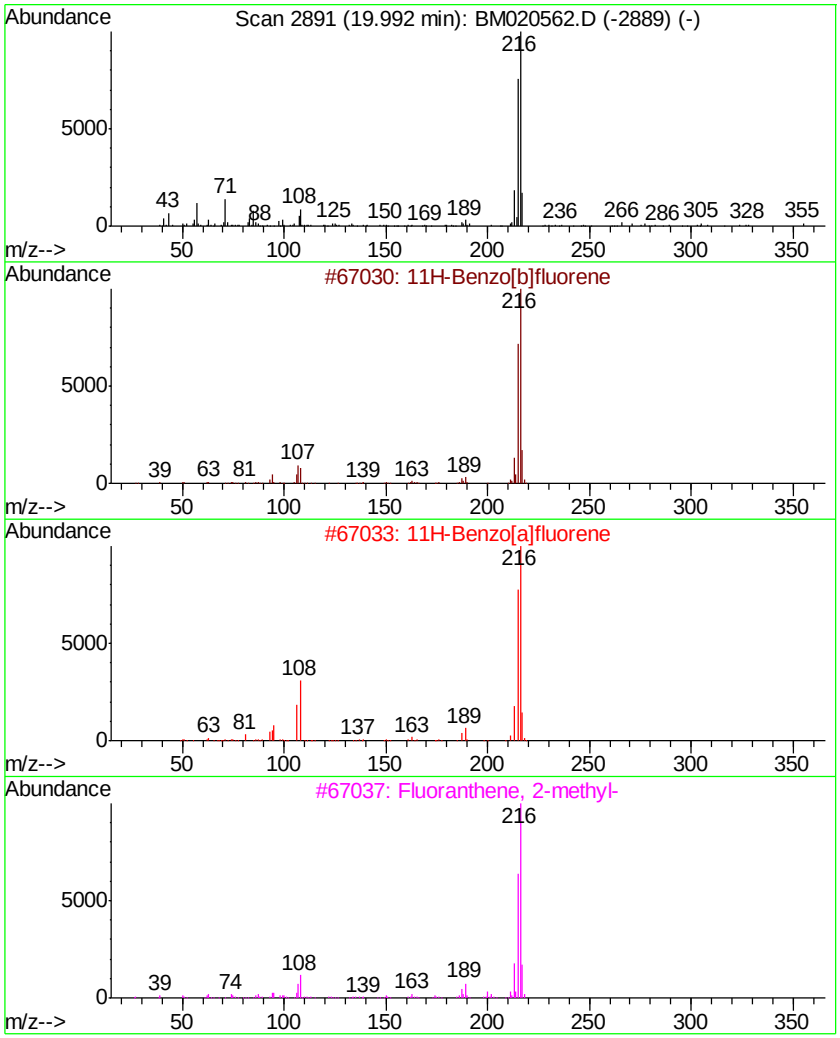
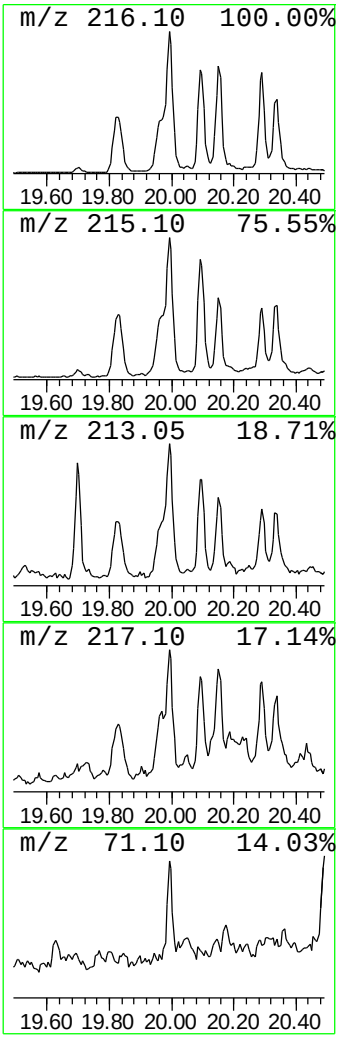
Peak Number 11 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.99	2.06 ng	232238	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	78
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	78
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	78
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM052419\
Data File : BM020562.D
Acq On : 25 May 2019 03:56
Operator : JU/SJ
Sample : K2647-11 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SU-03-052219-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM052419.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
unknown7.19	7.19	43.7	ng	921800	1	7.66	421609	20.0
Tridecanoic acid,...	17.73	6.8	ng	455035	4	17.07	1342600	20.0
Anthracene, 9-met...	17.94	3.3	ng	221922	4	17.07	1342600	20.0
Anthracene, 1-met...	17.99	3.3	ng	219334	4	17.07	1342600	20.0
4H-Cyclopenta[def...	18.14	4.4	ng	293605	4	17.07	1342600	20.0
7-Hexadecyne	18.87	24.2	ng	1621700	4	17.07	1342600	20.0
9-Octadecenoic ac...	18.91	31.1	ng	2086030	4	17.07	1342600	20.0
Octadecanoic acid...	19.04	6.5	ng	437649	4	17.07	1342600	20.0
Pyrene, 1-methyl-	19.83	2.3	ng	259036	5	21.26	2252720	20.0
11H-Benzo[b]fluorene	19.99	2.1	ng	232238	5	21.26	2252720	20.0