LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005693.D
Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B2(4-6)

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_P\Methods\8270E-BP052721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005693.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	9	11	18	rVB	97715	125038	1.83%	0.231%
2	4.469	230	235	242	rBV	84578	122431	1.79%	0.226%
3	5.075	331	338	347	rVB2	124719	192508	2.81%	0.356%
4	5.546	411	418	427	rBV	2002664	2947509	43.09%	5.451%
5	7.146	681	690	700	rBV	2003013	3182821	46.53%	5.886%
6	7.587	761	765	772	rBV	39157	77065	1.13%	0.143%
7	7.981	825	832	841	rBV	712003	1123879	16.43%	2.079%
8	9.146	1021	1030	1039	rBV	1238576	2048260	29.94%	3.788%
9	10.787	1302	1309	1316	rBV	886377	1505948	22.01%	2.785%
10	13.234	1717	1725	1737	rBV	3251467	4692932	68.60%	8.679%
11	13.504	1765	1771	1781	rBV	146378	233701	3.42%	0.432%
12	14.057	1857	1865	1871	rBV	292010	427902	6.26%	0.791%
13	14.604	1950	1958	1965	rBV	1345989	1929364	28.20%	3.568%
14	14.669	1965	1969	1976	rVB	45865	71142	1.04%	0.132%
15	15.222	2050	2063	2069	rBV4	28854	116044	1.70%	0.215%
16	15.645	2130	2135	2140	rBV	49034	78397	1.15%	0.145%
17	16.086	2204	2210	2219	rBV	2355474	3470362	50.73%	6.418%
18	17.110	2375	2384	2390	rBV9	48738	127753	1.87%	0.236%
19	17.169	2390	2394	2402	rVB	46180	77562	1.13%	0.143%
20	17.351	2418	2425	2428	rBV	1553578	2213800	32.36%	4.094%
21	17.392	2428	2432	2438	rVB	862834	1195548	17.48%	2.211%
22	17.481	2443	2447	2452	rVB	206958	286109	4.18%	0.529%
23	17.745	2489	2492	2499	rVB	56063	75302	1.10%	0.139%
24	18.210	2567	2571	2575	rBV	157163	208294	3.04%	0.385%
25	18.257	2575	2579	2584	rVB	193974	262889	3.84%	0.486%
26	18.339	2589	2593	2597	rVV	66021	91281	1.33%	0.169%
27	18.398	2598	2603	2607	rVV2	226290	410182	6.00%	0.759%
28	18.433	2607	2609	2614	rVB	108611	126567	1.85%	0.234%
29	18.692	2649	2653	2656	rBV	108590	140244	2.05%	0.259%
30	18.727	2656	2659	2667	rVB2	62186	91758	1.34%	0.170%
31	19.098	2718	2722	2728	rBV2	89632	171174	2.50%	0.317%
32	19.227	2741	2744	2751	rBV3	72461	118863	1.74%	0.220%
33	19.351	2759	2765	2770	rBV	1991566	2537120	37.09%	4.692%
34	19.486	2785	2788	2792	rBV4	63691	84118	1.23%	0.156%
35	19.669	2815	2819	2820	rBV	331345	368493	5.39%	0.681%
36	19.698	2820	2824	2832	rVB	1763850	2395342	35.02%	4.430%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
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Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B2(4-6)

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_P\Methods\8270E-BP052721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.769	2833	2836	2840	rVB2	75499	97715	1.43%	0.181%
38	19.892	2851	2857	2862	rBV	5710608	6840585	100.00%	12.651%
39	20.010	2873	2877	2878	rBV	101066	138612	2.03%	0.256%
40	20.180	2903	2906	2911	rVB2	282297	367211	5.37%	0.679%
41	20.274	2919	2922	2926	rBV	154155	190271	2.78%	0.352%
42	20.469	2952	2955	2958	rBV3	101085	129545	1.89%	0.240%
43	20.516	2960	2963	2966	rVB	96015	120653	1.76%	0.223%
44	20.904	3027	3029	3035	rVB	134704	167962	2.46%	0.311%
45	21.122	3061	3066	3075	rBV4	477872	1023304	14.96%	1.893%
46	21.416	3109	3116	3120	rBV2	2394907	4219340	61.68%	7.803%
47	21.457	3120	3123	3132	rVB	873957	1130989	16.53%	2.092%
48	23.110	3399	3404	3409	rBV	691539	1599950	23.39%	2.959%
49	23.639	3491	3494	3504	rVB	445614	834769	12.20%	1.544%
50	23.745	3507	3512	3521	rVB	673821	1306004	19.09%	2.415%
51	23.857	3525	3531	3538	rVV2	1272831	2576724	37.67%	4.765%

Sum of corrected areas: 54071336

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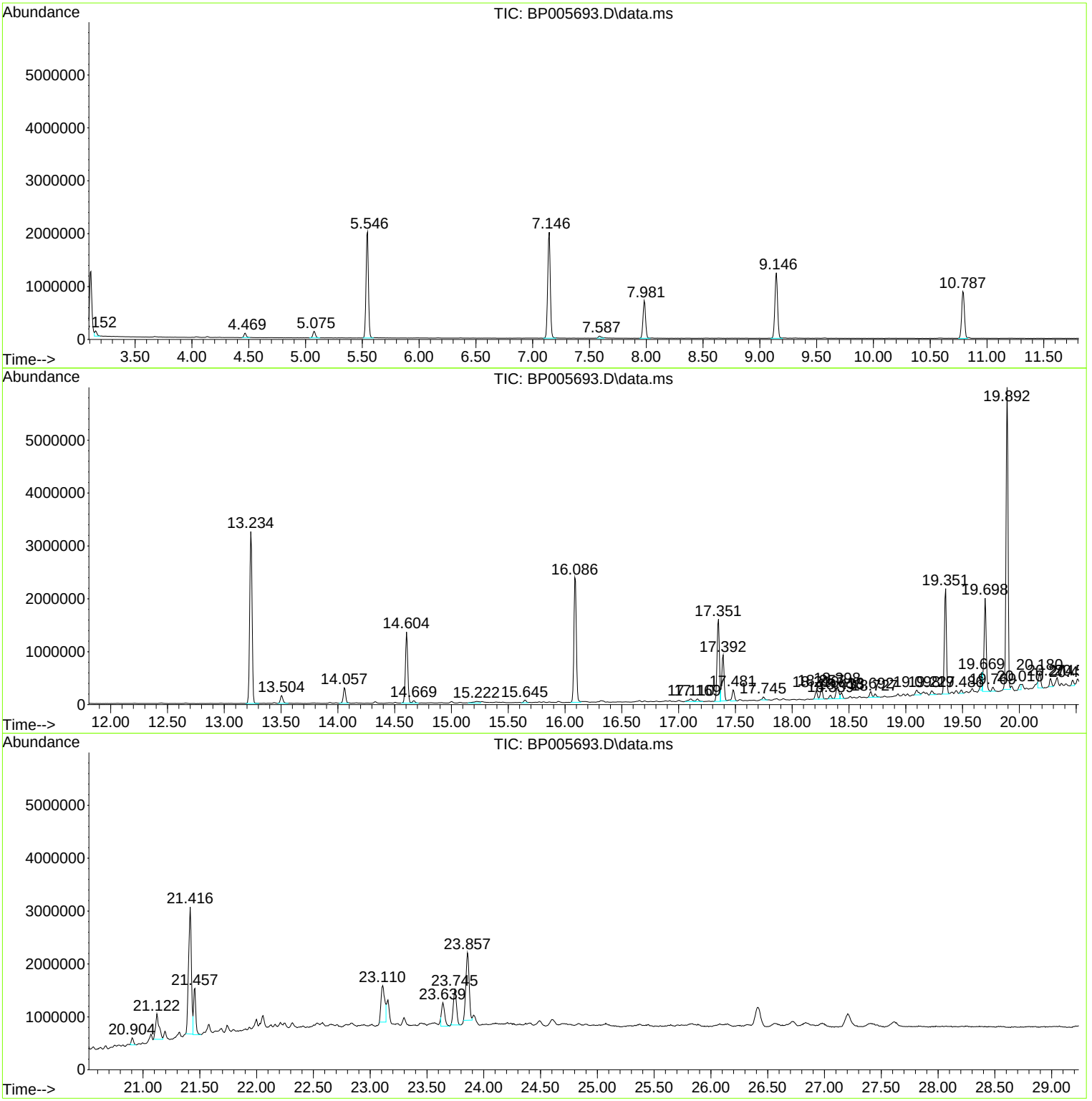
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005693.D
Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

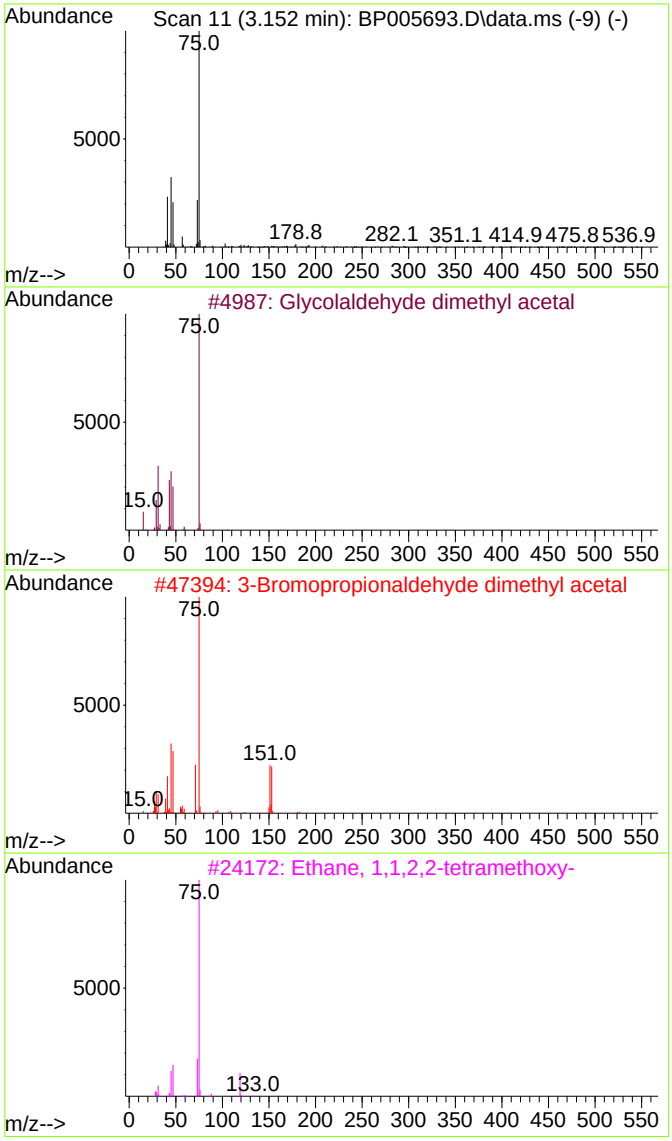
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

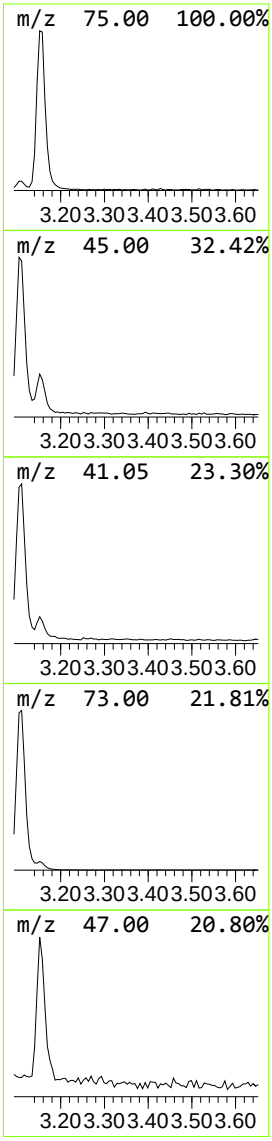
****

Peak Number 1 unknown3.152 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	2.23 ng	125038	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
2	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	45
3	Ethane, 1,1,2,2-tetramethoxy-	150	C6H14O4	002517-44-4	39
4	4-Methylvaleric acid, trimethyls...	188	C9H20O2Si	959048-10-3	39
5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

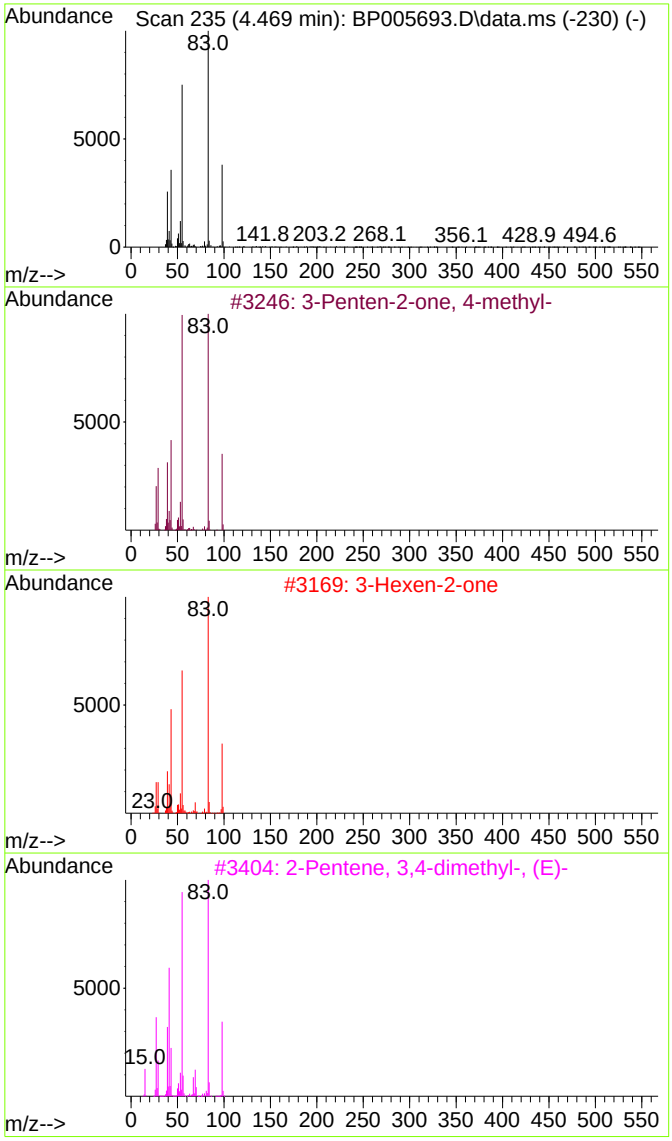
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

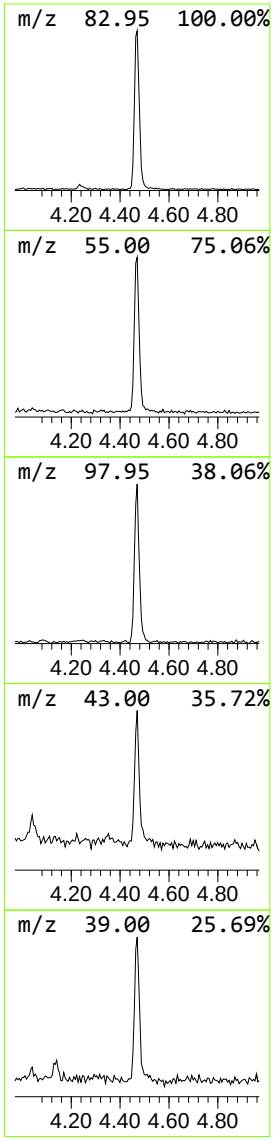
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	2.18 ng	122431	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	83
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	74





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Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B2(4-6)

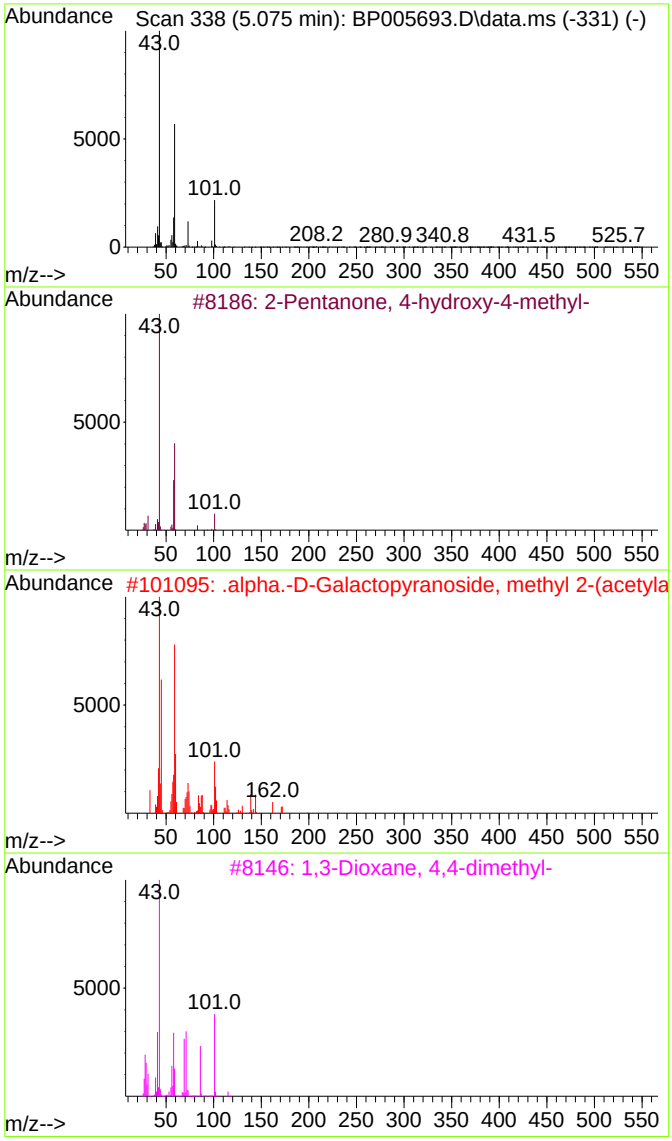
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

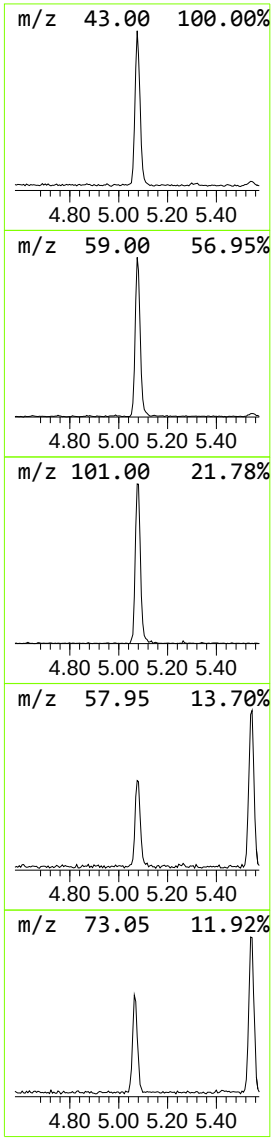
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.43 ng	192508	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	25
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

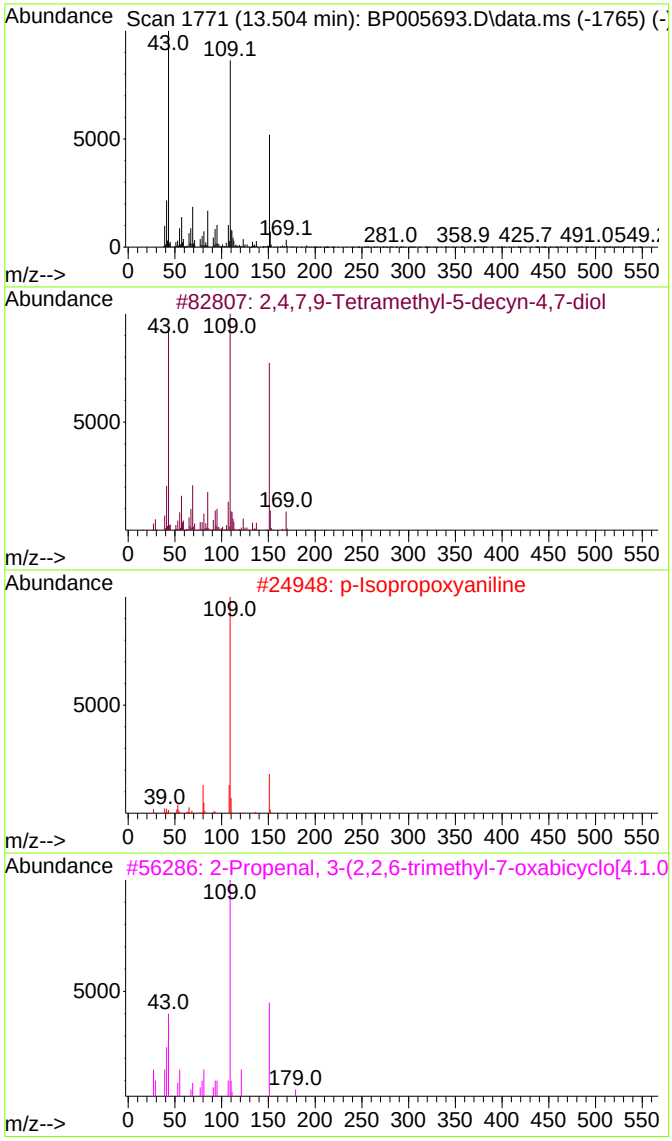
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

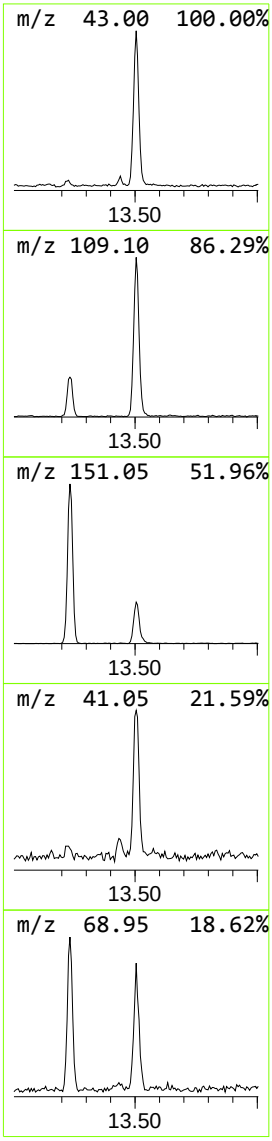
****

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	2.42 ng	233701	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	59
3	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
5	Cyclopentanol, 1-(methylenecyclo...	138	C9H14O	086951-58-8	46





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Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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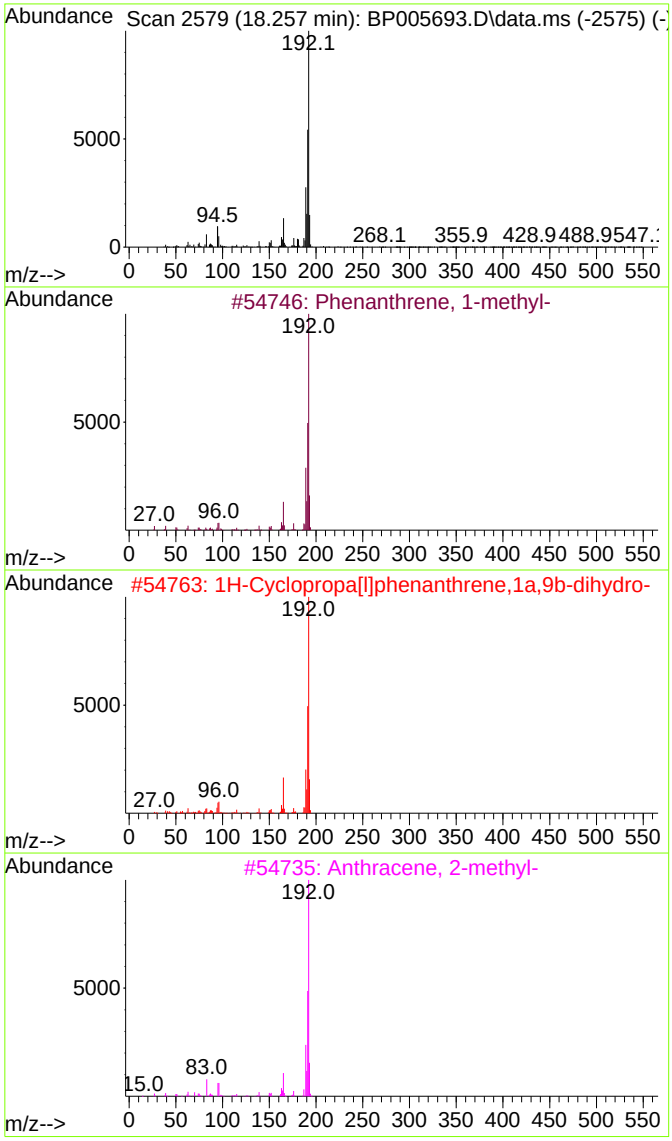
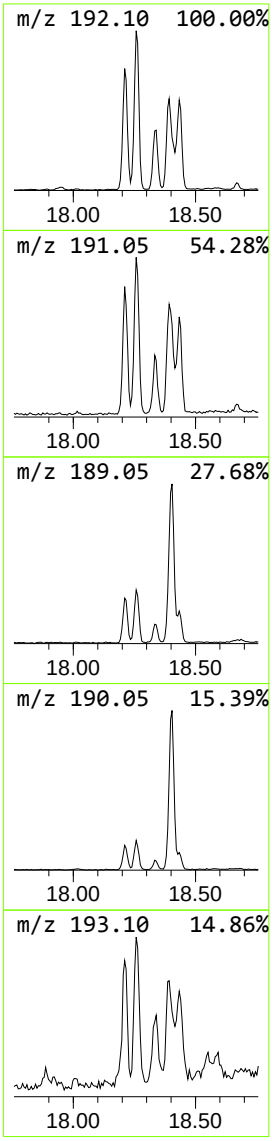
****

Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	2.38 ng	262889	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94





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Acq On : 03 Jun 2021 18:40
Operator : CG/JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.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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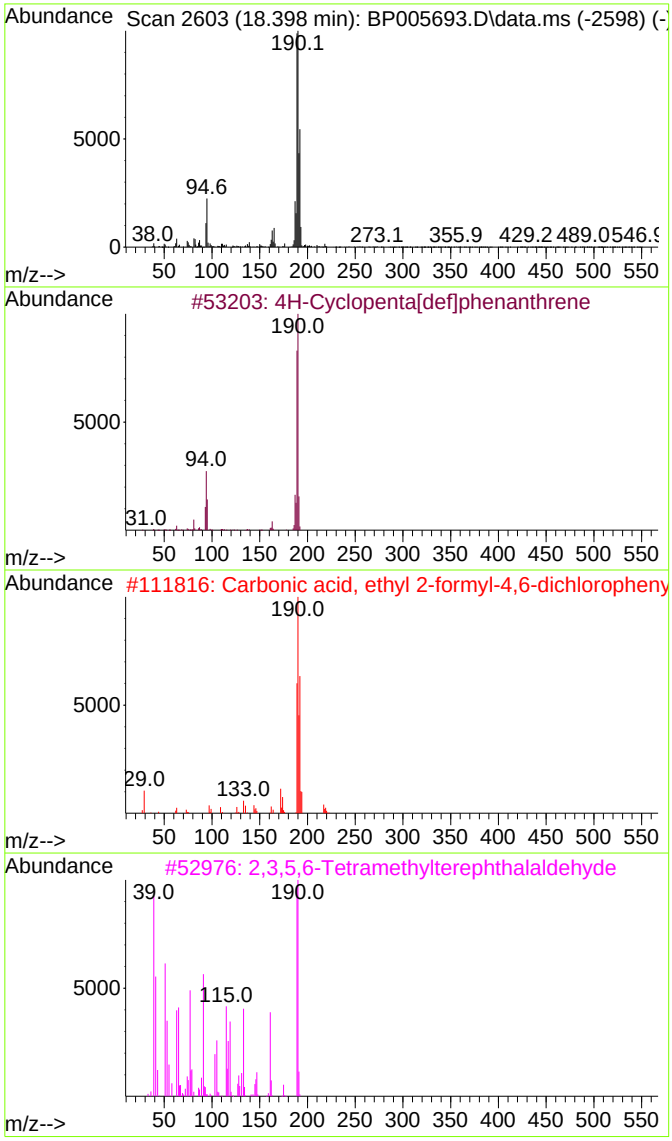
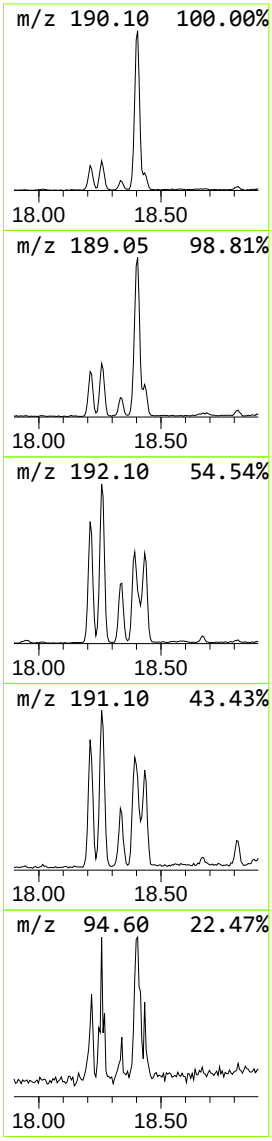
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	3.71 ng	410182	Phenanthrene-d10	17.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	25
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	18





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Instrument : BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.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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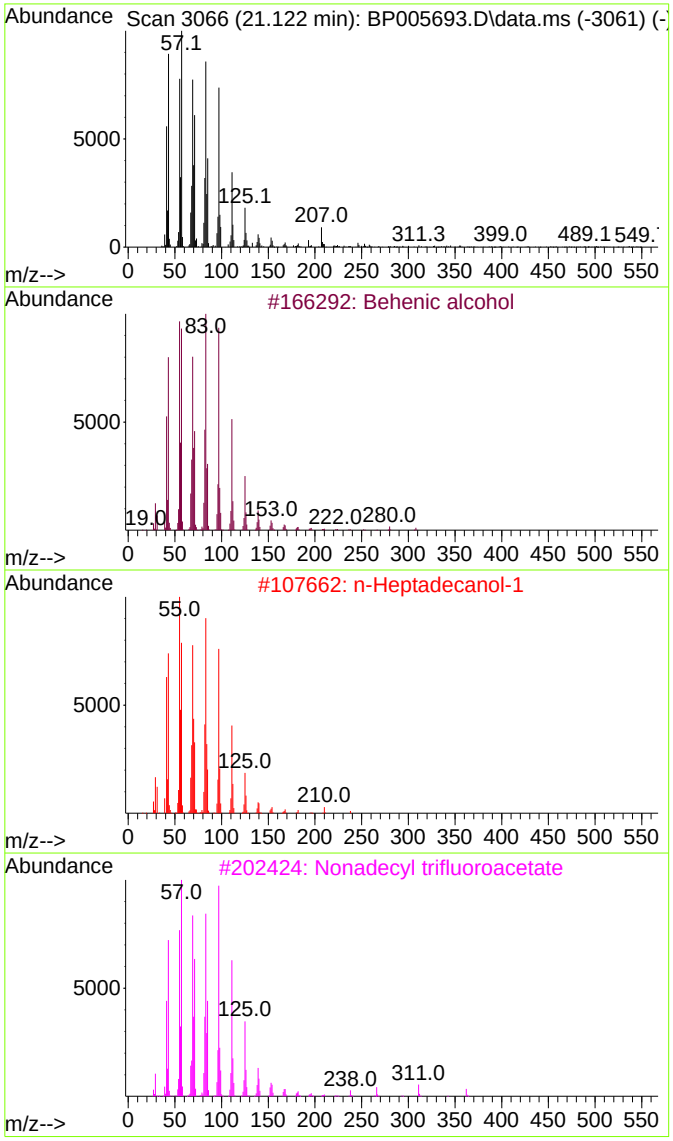
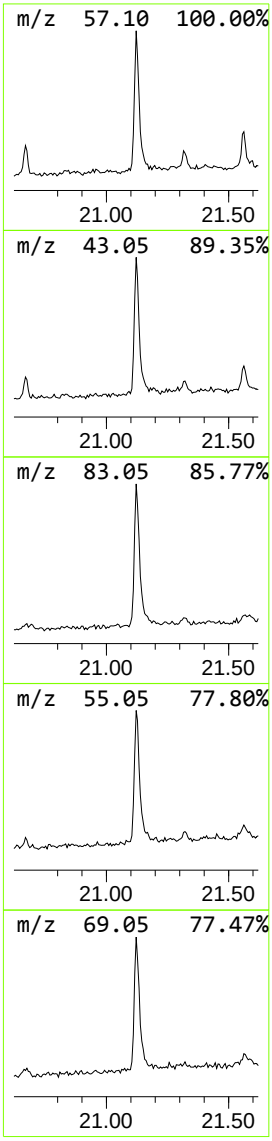
Peak Number 7 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	4.85 ng	1023300	Chrysene-d12	21.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
4	1-Heptacosanol	396	C27H56O	002004-39-9	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005693.D
Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.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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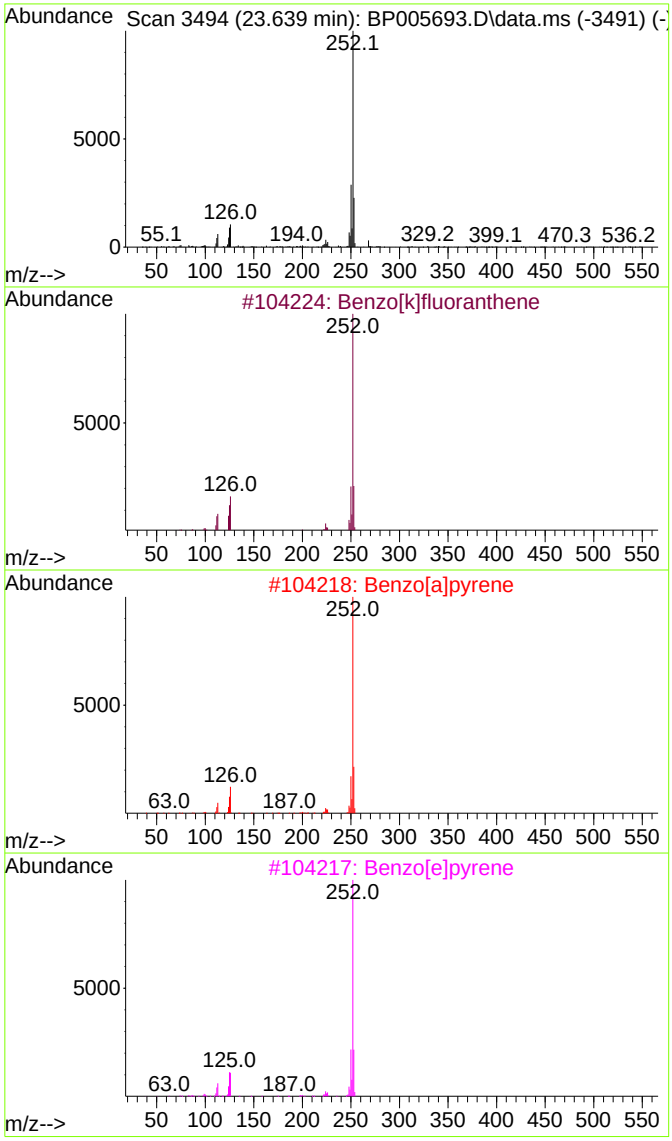
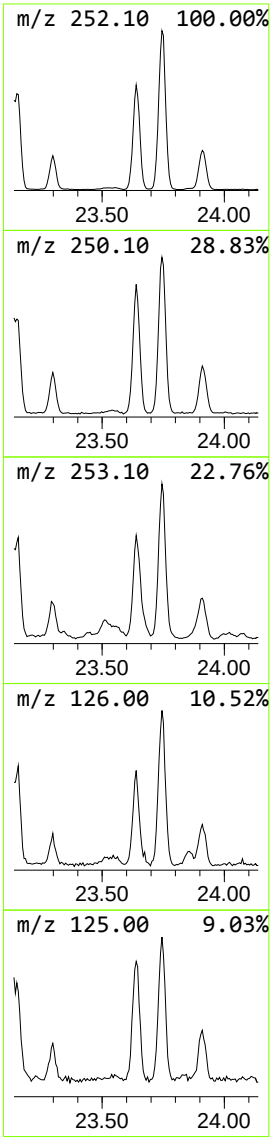
Peak Number 8 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.639	6.48 ng	834769	Perylene-d12	23.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005693.D
Acq On : 03 Jun 2021 18:40
Operator : CG/JU
Sample : M2580-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B2(4-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.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
unknown3.152	3.152	2.2	ng	125038	1	7.981	1123880	20.0
3-Penten-2-one,...	4.469	2.2	ng	122431	1	7.981	1123880	20.0
2-Pentanone, 4-...	5.075	3.4	ng	192508	1	7.981	1123880	20.0
2,4,7,9-Tetrame...	13.504	2.4	ng	233701	3	14.604	1929360	20.0
Phenanthrene, 1...	18.257	2.4	ng	262889	4	17.351	2213800	20.0
4H-Cyclopenta[d...	18.398	3.7	ng	410182	4	17.351	2213800	20.0
Behenic alcohol	21.122	4.8	ng	1023300	5	21.416	4219340	20.0
Benzo[e]pyrene	23.639	6.5	ng	834769	6	23.857	2576720	20.0