LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

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\8270-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003461.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.664	297	302	313	rBV	44214	71125	1.61%	0.219%
2	5.140	377	383	411	rBV	971060	1693435	38.28%	5.220%
3	6.734	647	654	690	rBV	836434	1732575	39.17%	5.340%
4	7.528	781	789	800	rBV	390229	657114	14.85%	2.025%
5	8.681	977	985	1014	rBV	593318	1252734	28.32%	3.861%
6	10.304	1254	1261	1299	rBV	393930	969322	21.91%	2.988%
7	12.798	1678	1685	1711	rBV	1492039	2986816	67.52%	9.206%
8	13.651	1825	1830	1843	rBV	101322	211126	4.77%	0.651%
9	14.187	1914	1921	1929	rBV	721733	1237738	27.98%	3.815%
10	15.692	2170	2177	2201	rBV	972455	1936010	43.76%	5.967%
11	15.934	2214	2218	2230	rVB8	21725	47040	1.06%	0.145%
12	16.945	2384	2390	2394	rBV	961822	1461550	33.04%	4.505%
13	16.986	2394	2397	2404	rVB	192577	280793	6.35%	0.865%
14	17.081	2409	2413	2420	rVB	49206	79238	1.79%	0.244%
15	17.822	2534	2539	2543	rBV	56998	82287	1.86%	0.254%
16	17.875	2543	2548	2553	rVB	78682	112975	2.55%	0.348%
17	18.010	2566	2571	2575	rBV2	132880	208126	4.70%	0.642%
18	18.045	2575	2577	2586	rVB	43321	59540	1.35%	0.184%
19	18.310	2618	2622	2627	rBV	38425	54540	1.23%	0.168%
20	18.363	2627	2631	2636	rVB2	39255	53389	1.21%	0.165%
21	18.716	2686	2691	2696	rBV	75572	121647	2.75%	0.375%
22	18.781	2696	2702	2705	rVV4	36710	71475	1.62%	0.220%
23	18.863	2710	2716	2722	rBV2	84687	155089	3.51%	0.478%
24	18.969	2729	2734	2741	rBV	926538	1150449	26.01%	3.546%
25	19.322	2785	2794	2799	rBV	805266	1209713	27.35%	3.729%
26	19.404	2804	2808	2815	rVB3	50668	75066	1.70%	0.231%
27	19.528	2822	2829	2834	rBV	3483040	4423738	100.00%	13.635%
28	19.645	2844	2849	2857	rBV3	75363	185021	4.18%	0.570%
29	19.780	2867	2872	2874	rBV3	66595	114079	2.58%	0.352%
30	19.810	2874	2877	2881	rVB	124091	172536	3.90%	0.532%
31	19.910	2890	2894	2898	rBV	104373	124508	2.81%	0.384%
32	19.963	2898	2903	2907	rBV2	111212	178017	4.02%	0.549%
33	20.104	2923	2927	2931	rBV2	76107	104662	2.37%	0.323%
34	20.145	2931	2934	2939	rVB2	58574	84117	1.90%	0.259%
35	20.551	2999	3003	3007	rVB	71903	91142	2.06%	0.281%
36	20.704	3026	3029	3032	rBV	84723	109083	2.47%	0.336%

LSC Area Percent Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

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\8270-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.733	3032	3034	3037	rVV2	84612	90253	2.04%	0.278%
38	20.775	3037	3041	3047	rVV3	538329	822008	18.58%	2.534%
39	20.833	3047	3051	3057	rVB2	169123	298497	6.75%	0.920%
40	20.969	3072	3074	3077	rVB	55643	50559	1.14%	0.156%
41	21.045	3081	3087	3091	rVV2	1512197	2329881	52.67%	7.181%
42	21.080	3091	3093	3099	rVB	324246	402681	9.10%	1.241%
43	21.204	3110	3114	3117	rBV2	103221	132390	2.99%	0.408%
44	21.586	3177	3179	3182	rVB	67952	67888	1.53%	0.209%
45	21.645	3183	3189	3195	rBV5	145785	355242	8.03%	1.095%
46	22.069	3258	3261	3266	rBV4	93542	136911	3.09%	0.422%
47	22.198	3280	3283	3292	rVB2	75445	136111	3.08%	0.420%
48	22.298	3297	3300	3303	rVB3	56170	69687	1.58%	0.215%
49	22.574	3342	3347	3352	rBV2	334150	707668	16.00%	2.181%
50	23.045	3423	3427	3434	rVB	150504	240135	5.43%	0.740%
51	23.139	3437	3443	3451	rVB	181534	346063	7.82%	1.067%
52	23.233	3452	3459	3465	rBV2	936662	1756351	39.70%	5.414%
53	23.757	3543	3548	3556	rVB	167025	332552	7.52%	1.025%
54	23.851	3559	3564	3574	rVV5	76223	218689	4.94%	0.674%
55	26.221	3961	3967	3985	rVB9	114940	392171	8.87%	1.209%

Sum of corrected areas: 32443552

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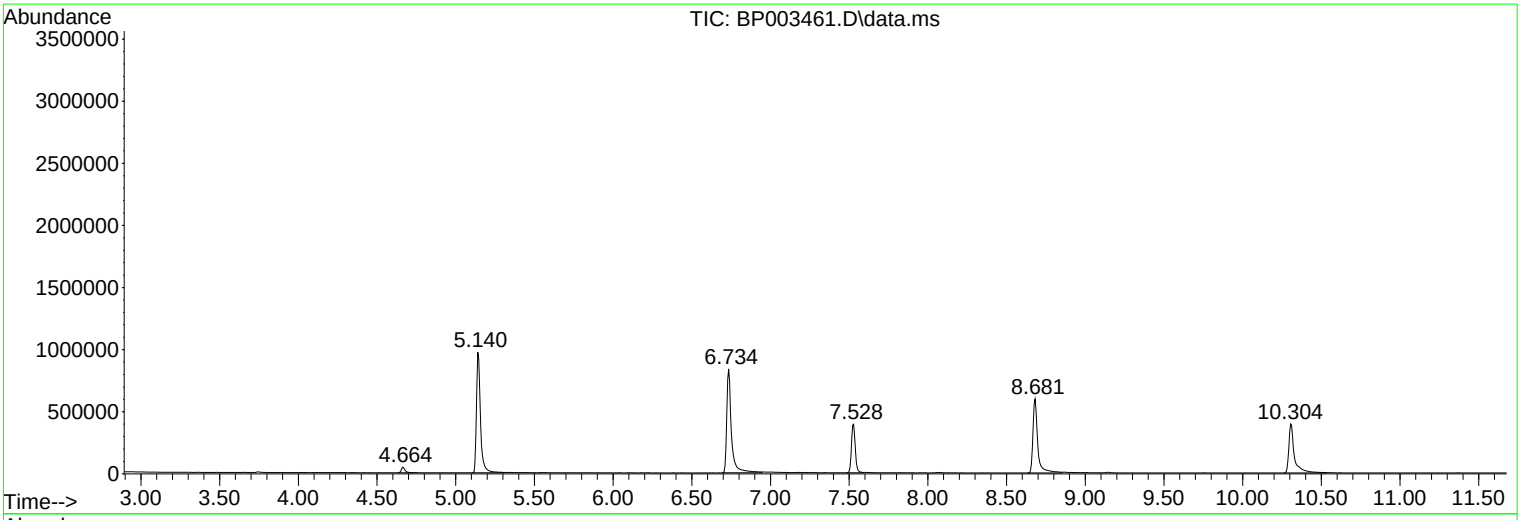
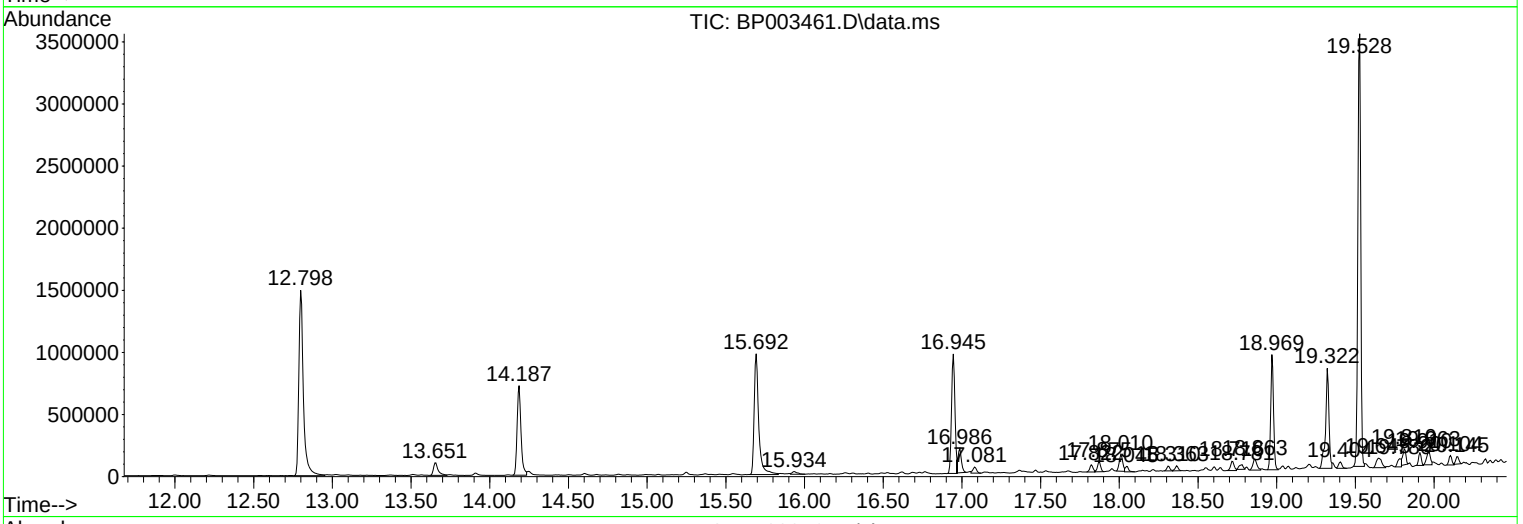
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

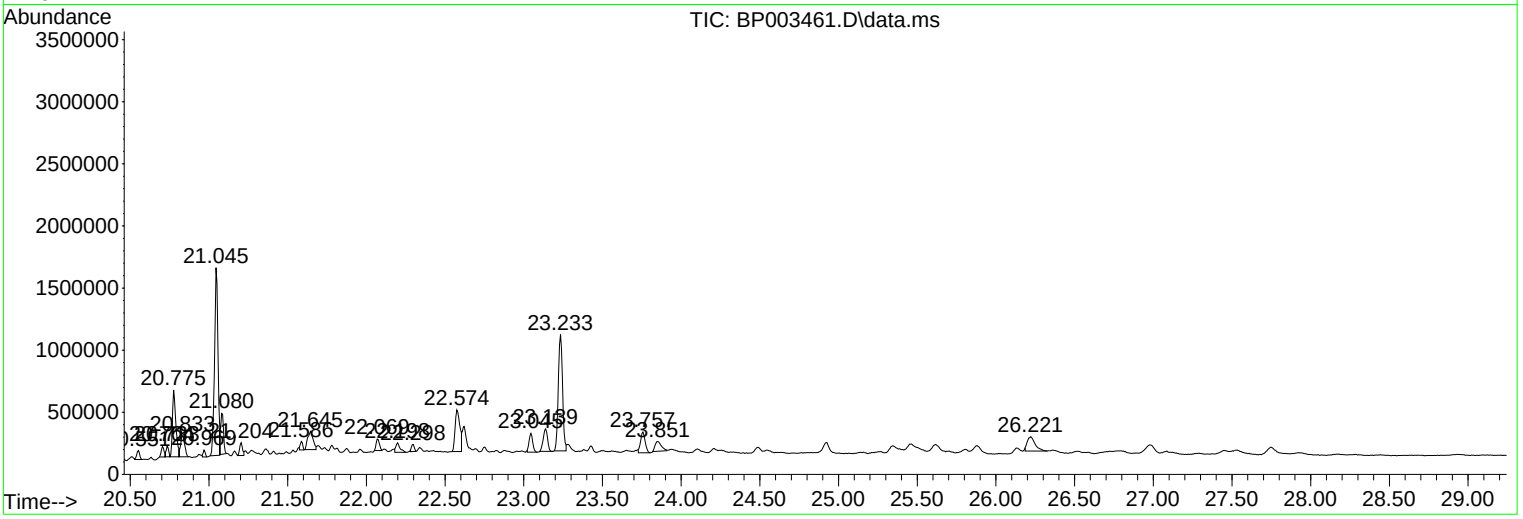
Instrument :
BNA_P
ClientSampleId :
RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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Sample : L4198-16
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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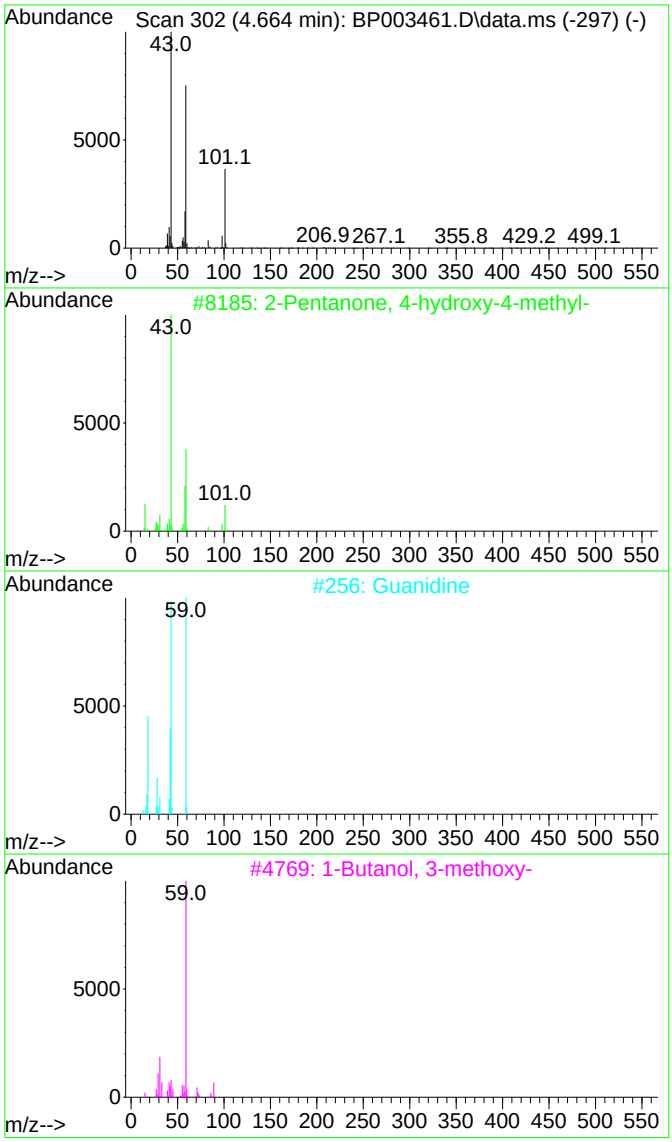
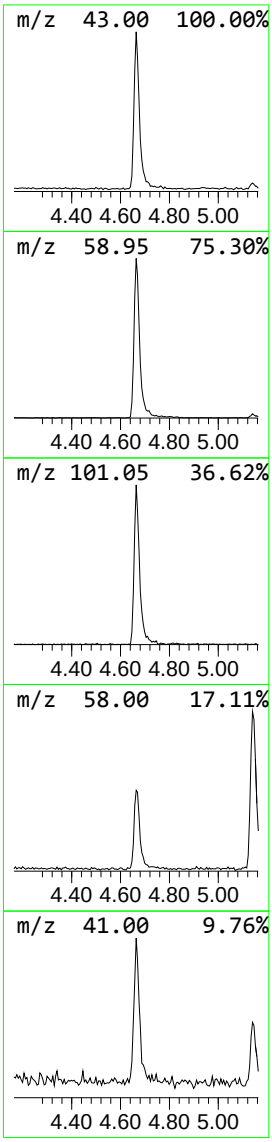
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.664	2.16 ng	71125	1,4-Dichlorobenzene-d4	7.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	50
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	37
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	36
5	Dimethadione	129	C5H7NO3	000695-53-4	36





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Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

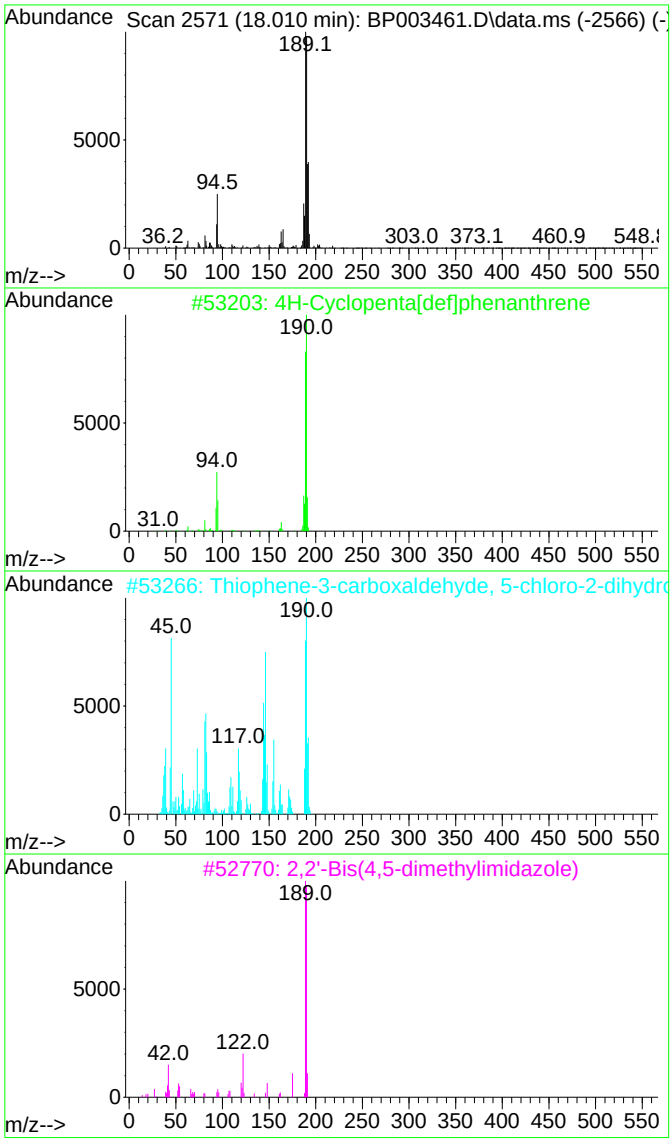
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

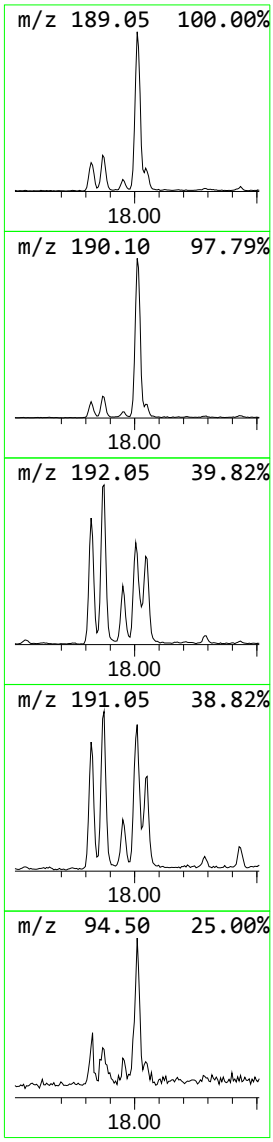
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	2.85 ng	208126	Phenanthrene-d10	16.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	1-Aminocyclopentanecarboxylic ac...	361	C18H32ClNO4	1000329-17-0	17





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Instrument :
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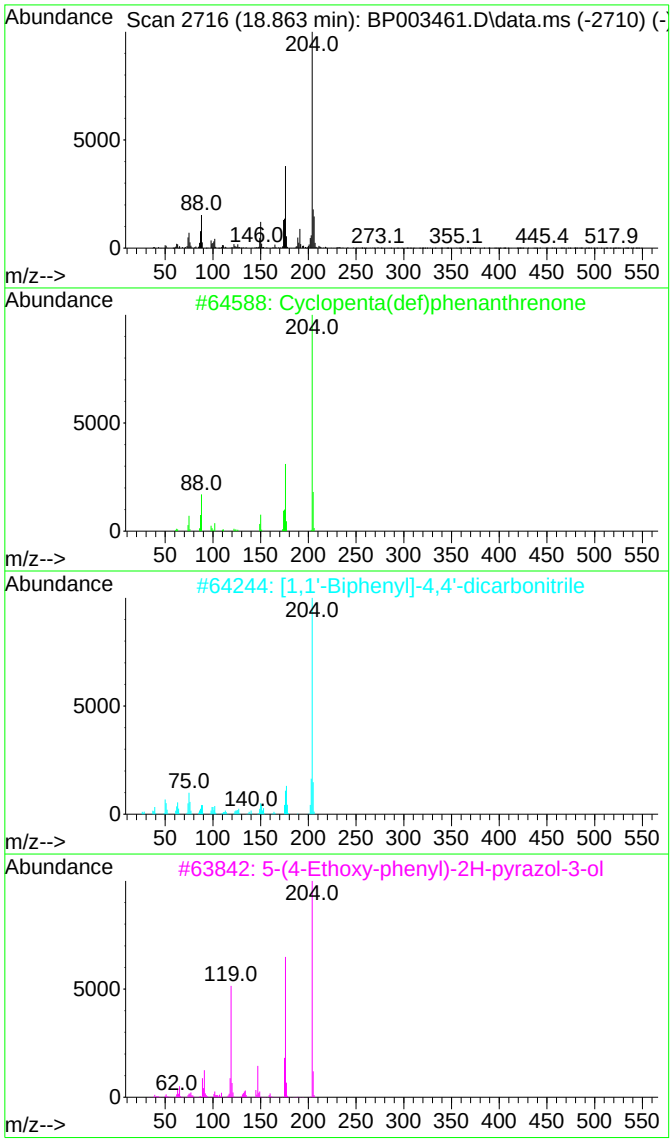
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

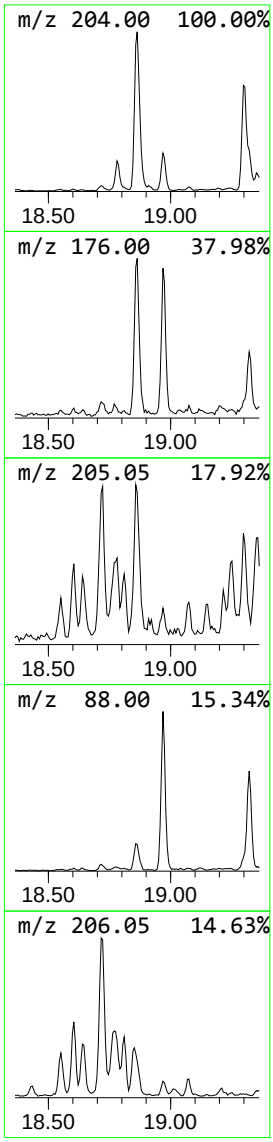
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopenta(def)phenanthrenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.863	2.12 ng	155089	Phenanthrene-d10	16.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	96
2	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	59
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	58
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
5	Benzo[1,2-b:4,3-b']dithiophene, ...	204	C11H8S2	013640-86-3	47





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Instrument : BNA_P
ClientSampleId : RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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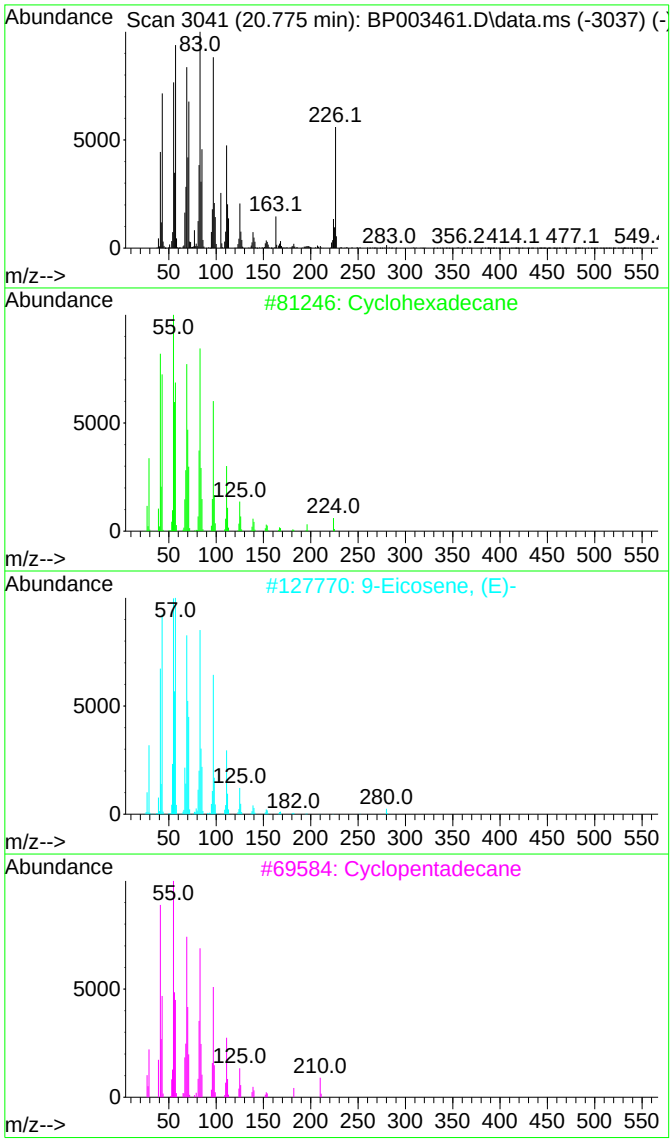
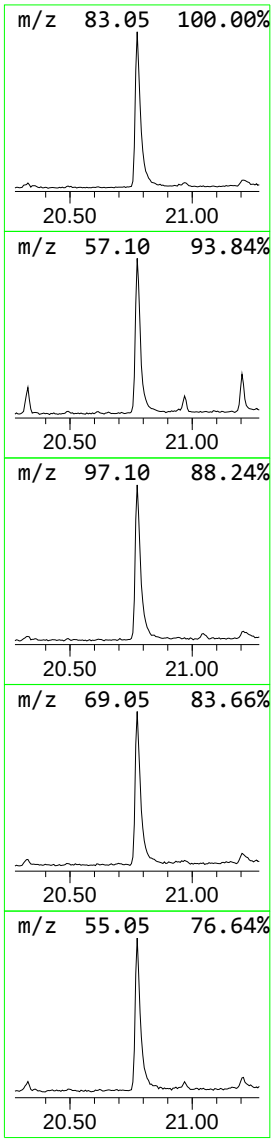
****

Peak Number 4 Cyclohexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.775	7.06 ng	822008	Chrysene-d12	21.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	93
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	Cyclopentadecane	210	C15H30	000295-48-7	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





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Operator : CG/JU
Sample : L4198-16
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ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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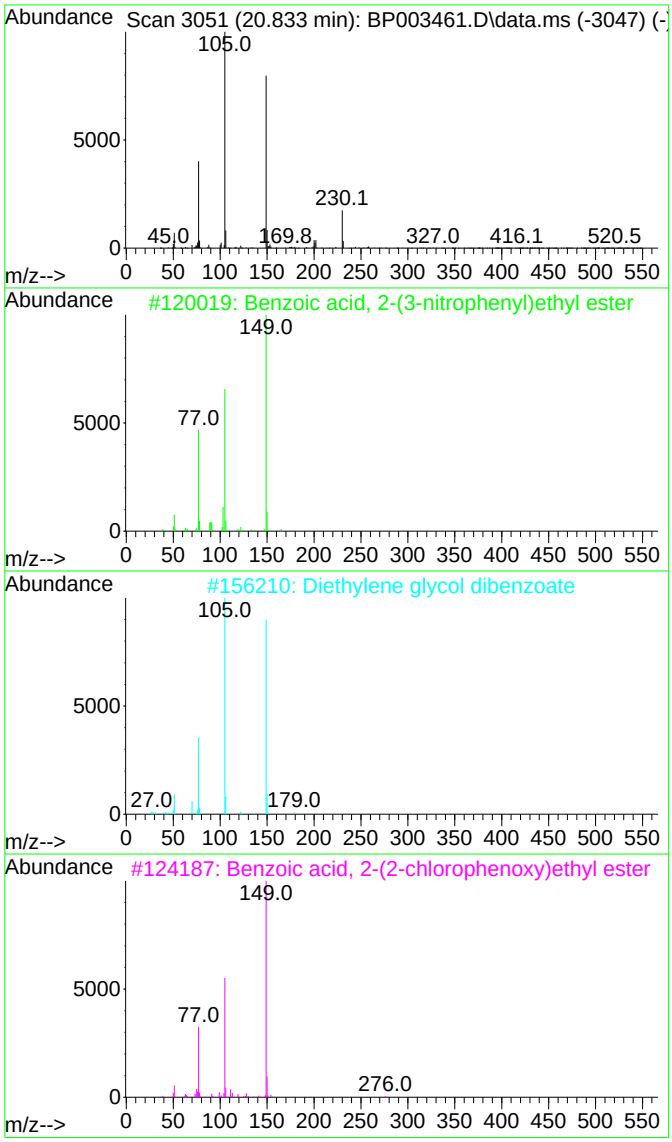
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

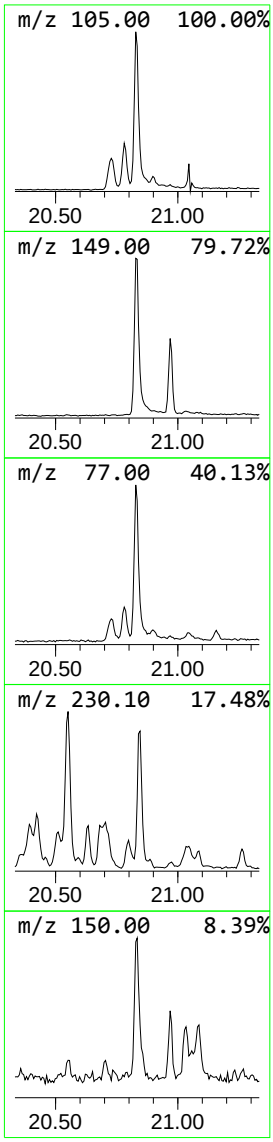
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, 2-(3-nitrophe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.833	2.56 ng	298497	Chrysene-d12	21.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
3	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
5	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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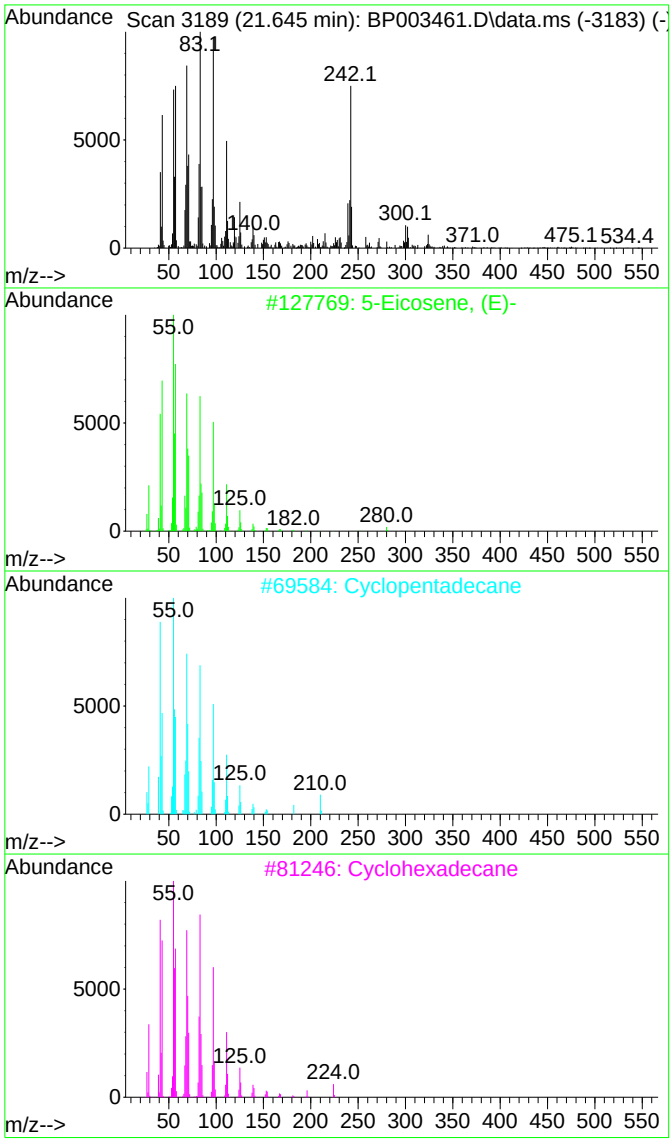
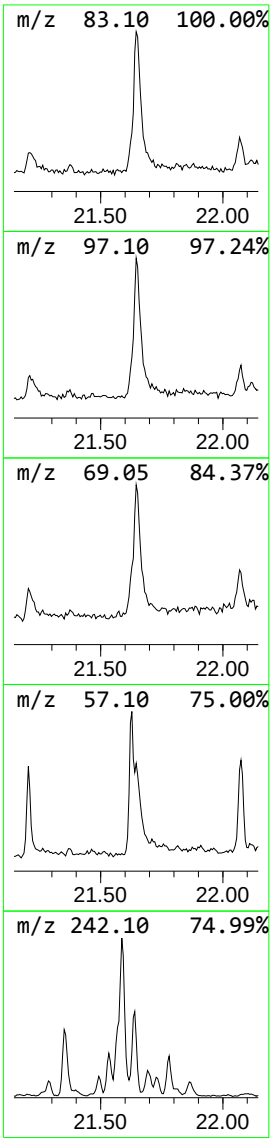
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.645	3.05 ng	355242	Chrysene-d12	21.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Cyclopentadecane	210	C15H30	000295-48-7	90
3	Cyclohexadecane	224	C16H32	000295-65-8	89
4	1-Tricosene	322	C23H46	018835-32-0	83
5	1-Heptacosanol	396	C27H56O	002004-39-9	78





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Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

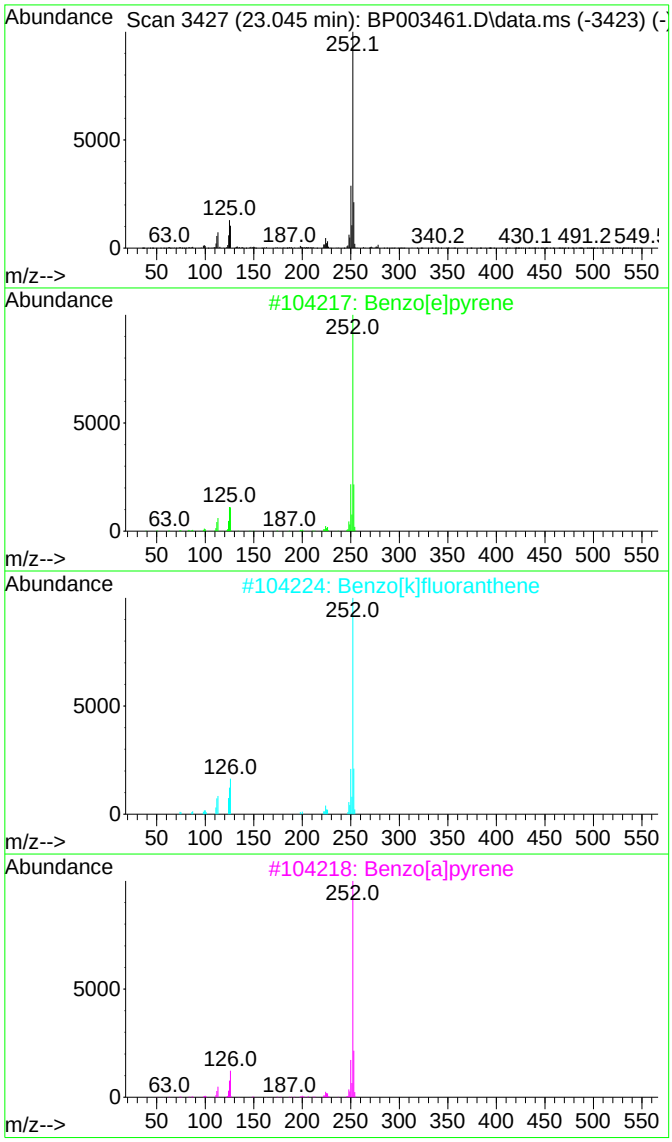
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

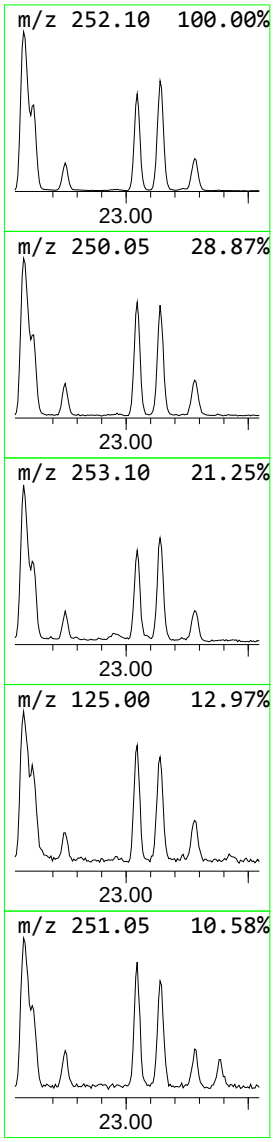
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.045	2.73 ng	240135	Perylene-d12	23.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Perylene	252	C20H12	000198-55-0	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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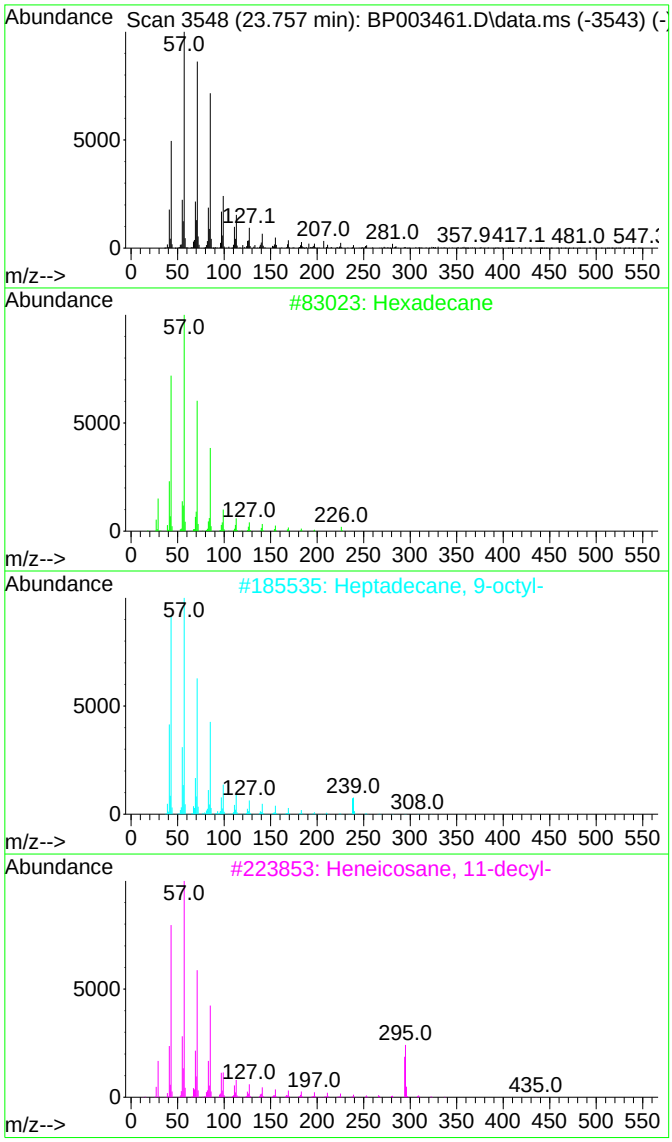
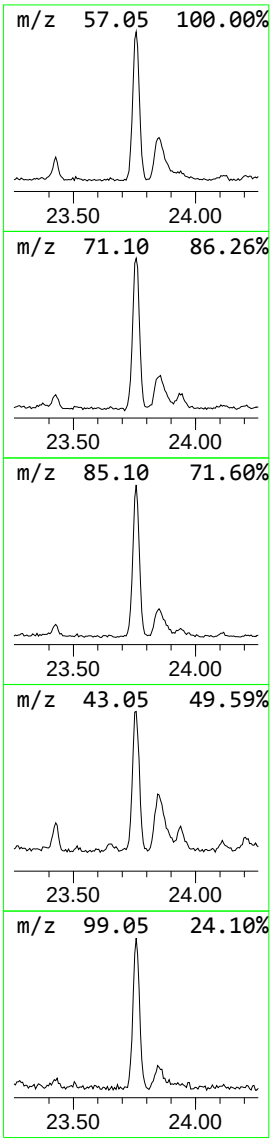
Peak Number 8 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.757	3.79 ng	332552	Perylene-d12	23.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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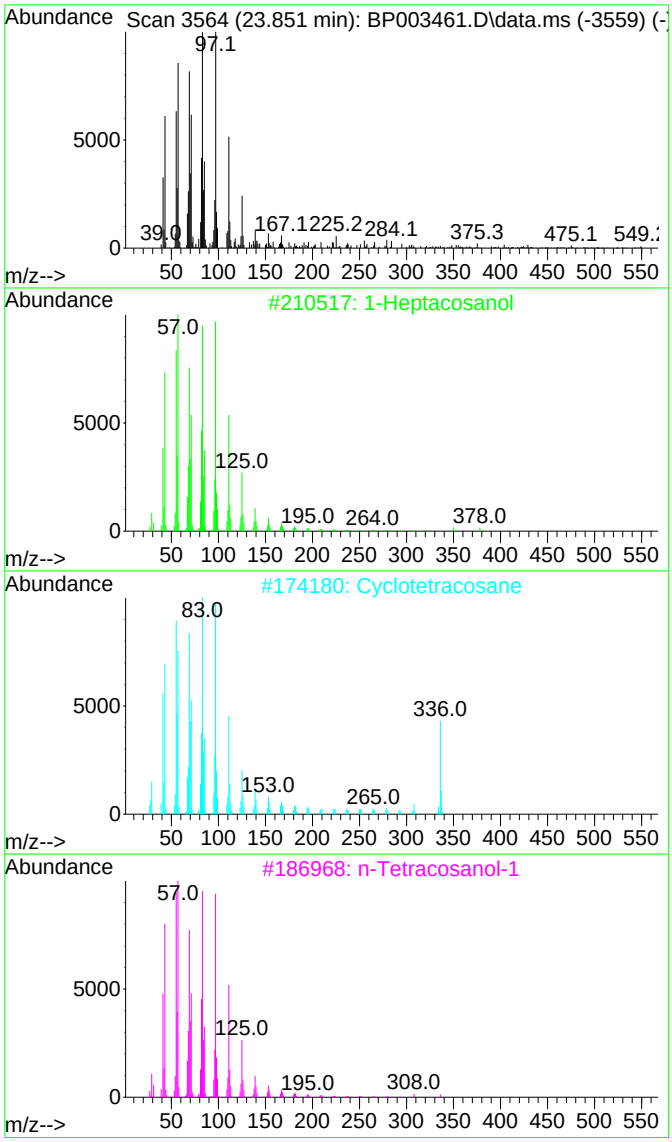
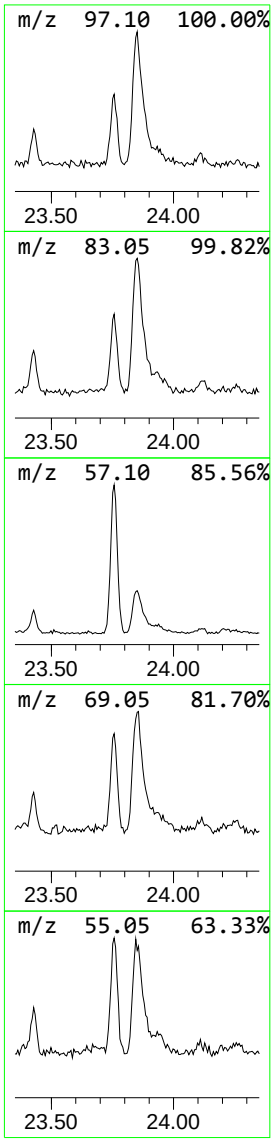
Peak Number 9 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.851	2.49 ng	218689	Perylene-d12	23.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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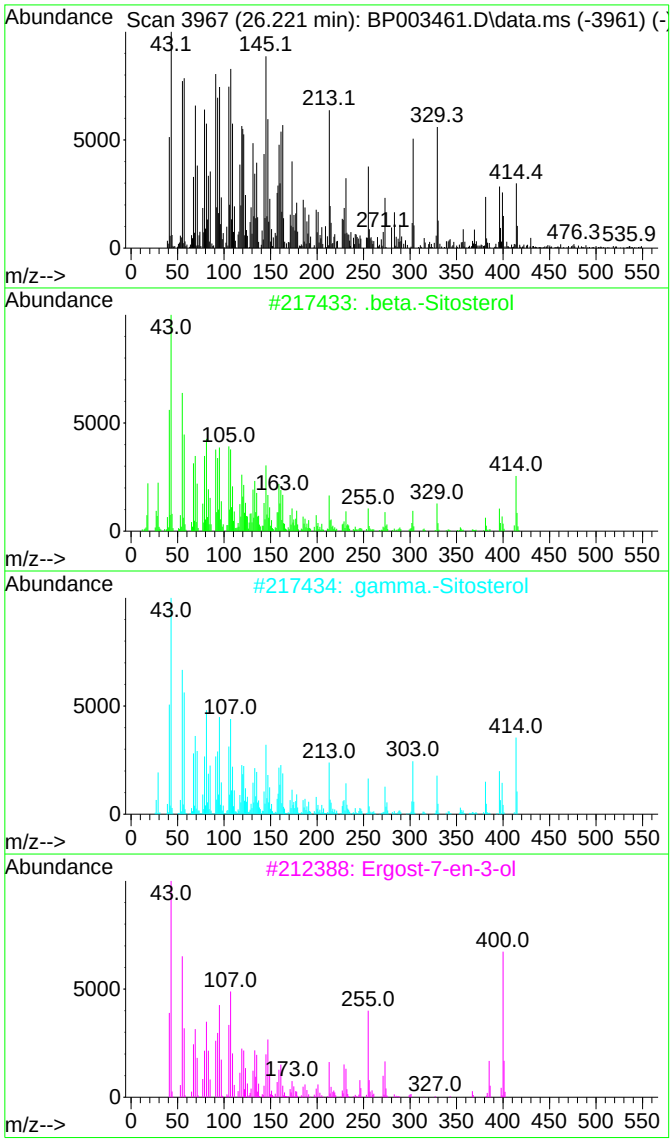
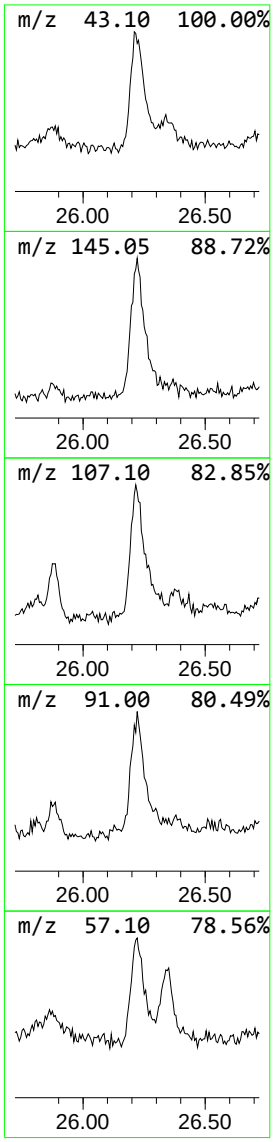
Peak Number 10 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.221	4.47 ng	392171	Perylene-d12	23.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	49
3	Ergost-7-en-3-ol	400	C28H48O	116179-22-7	42
4	Furan-2-carboxylic acid, (4-benz...	303	C19H13NO3	1000316-79-6	14
5	5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003461.D
Acq On : 02 Oct 2020 15:49
Operator : CG/JU
Sample : L4198-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RO-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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-...	4.664	2.2	ng	71125	1	7.528	657114	20.0
4H-Cyclopenta[d...	18.010	2.9	ng	208126	4	16.945	1461550	20.0
Cyclopenta(def)...	18.863	2.1	ng	155089	4	16.945	1461550	20.0
Cyclohexadecane	20.775	7.1	ng	822008	5	21.045	2329880	20.0
Benzoic acid, 2...	20.833	2.6	ng	298497	5	21.045	2329880	20.0
5-Eicosene, (E)-	21.645	3.0	ng	355242	5	21.045	2329880	20.0
Benzo[e]pyrene	23.045	2.7	ng	240135	6	23.233	1756350	20.0
Hexadecane	23.757	3.8	ng	332552	6	23.233	1756350	20.0
1-Heptacosanol	23.851	2.5	ng	218689	6	23.233	1756350	20.0
.beta.-Sitosterol	26.221	4.5	ng	392171	6	23.233	1756350	20.0