LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BS-SP2

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005479.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	368	375	388	rBV	184714	273099	29.20%	5.291%
2	6.899	641	648	660	rBV	151924	247082	26.41%	4.787%
3	7.705	778	785	791	rBV	51461	80087	8.56%	1.552%
4	8.869	975	983	996	rBV	98034	165051	17.64%	3.198%
5	10.493	1252	1259	1267	rBV2	49144	84108	8.99%	1.630%
6	12.969	1673	1680	1697	rBV	252374	372264	39.80%	7.213%
7	13.822	1820	1825	1835	rBV	10569	17079	1.83%	0.331%
8	14.345	1908	1914	1921	rBV	75822	111618	11.93%	2.163%
9	14.410	1921	1925	1935	rVB2	6241	9630	1.03%	0.187%
10	15.404	2088	2094	2100	rBV3	6536	10795	1.15%	0.209%
11	15.845	2160	2169	2179	rBV	284037	427880	45.74%	8.290%
12	17.098	2377	2382	2386	rBV	119179	163618	17.49%	3.170%
13	17.139	2386	2389	2396	rVV	70504	98793	10.56%	1.914%
14	17.234	2400	2405	2412	rVB	21229	31593	3.38%	0.612%
15	17.975	2526	2531	2533	rBV2	13193	20338	2.17%	0.394%
16	18.004	2533	2536	2537	rVV3	15828	20784	2.22%	0.403%
17	18.022	2537	2539	2545	rVV	20633	24685	2.64%	0.478%
18	18.104	2548	2553	2557	rVV2	6810	12465	1.33%	0.242%
19	18.157	2557	2562	2566	rVV3	22338	39802	4.25%	0.771%
20	18.192	2566	2568	2578	rVB	10140	14259	1.52%	0.276%
21	18.457	2609	2613	2619	rBV	10359	15113	1.62%	0.293%
22	18.504	2619	2621	2627	rVB7	7344	10444	1.12%	0.202%
23	18.863	2677	2682	2685	rBV2	10470	14898	1.59%	0.289%
24	19.010	2701	2707	2715	rBV2	5698	13992	1.50%	0.271%
25	19.116	2720	2725	2731	rBV	154533	191390	20.46%	3.708%
26	19.469	2776	2785	2794	rBV	127391	211903	22.65%	4.106%
27	19.545	2794	2798	2802	rVB4	7299	10428	1.11%	0.202%
28	19.669	2812	2819	2825	rBV	801609	935428	100.00%	18.124%
29	19.798	2834	2841	2846	rBV7	11934	27602	2.95%	0.535%
30	19.922	2858	2862	2863	rBV3	7650	9376	1.00%	0.182%
31	19.957	2864	2868	2872	rVB	26792	38591	4.13%	0.748%
32	20.051	2880	2884	2888	rBV	20645	27498	2.94%	0.533%
33	20.110	2890	2894	2898	rVB2	12805	18552	1.98%	0.359%
34	20.245	2914	2917	2921	rVB3	10858	12478	1.33%	0.242%
35	20.692	2991	2993	2998	rVB4	11043	10573	1.13%	0.205%
36	20.851	3017	3020	3022	rBV2	15670	20202	2.16%	0.391%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BS-SP2

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.880	3023	3025	3027	rVV2	18028	21126	2.26%	0.409%
38	20.910	3027	3030	3037	rVV7	33819	71375	7.63%	1.383%
39	20.980	3038	3042	3047	rVB2	40229	53552	5.72%	1.038%
40	21.192	3071	3078	3082	rBV2	291265	456359	48.79%	8.842%
41	21.227	3082	3084	3089	rVB	76118	85025	9.09%	1.647%
42	21.310	3095	3098	3101	rBV5	15549	21098	2.26%	0.409%
43	22.804	3347	3352	3357	rBV2	67263	149159	15.95%	2.890%
44	23.304	3433	3437	3446	rVB2	37429	70053	7.49%	1.357%
45	23.404	3449	3454	3460	rVB2	56793	108950	11.65%	2.111%
46	23.504	3465	3471	3478	rBV2	178170	331002	35.39%	6.413%

Sum of corrected areas: 5161197

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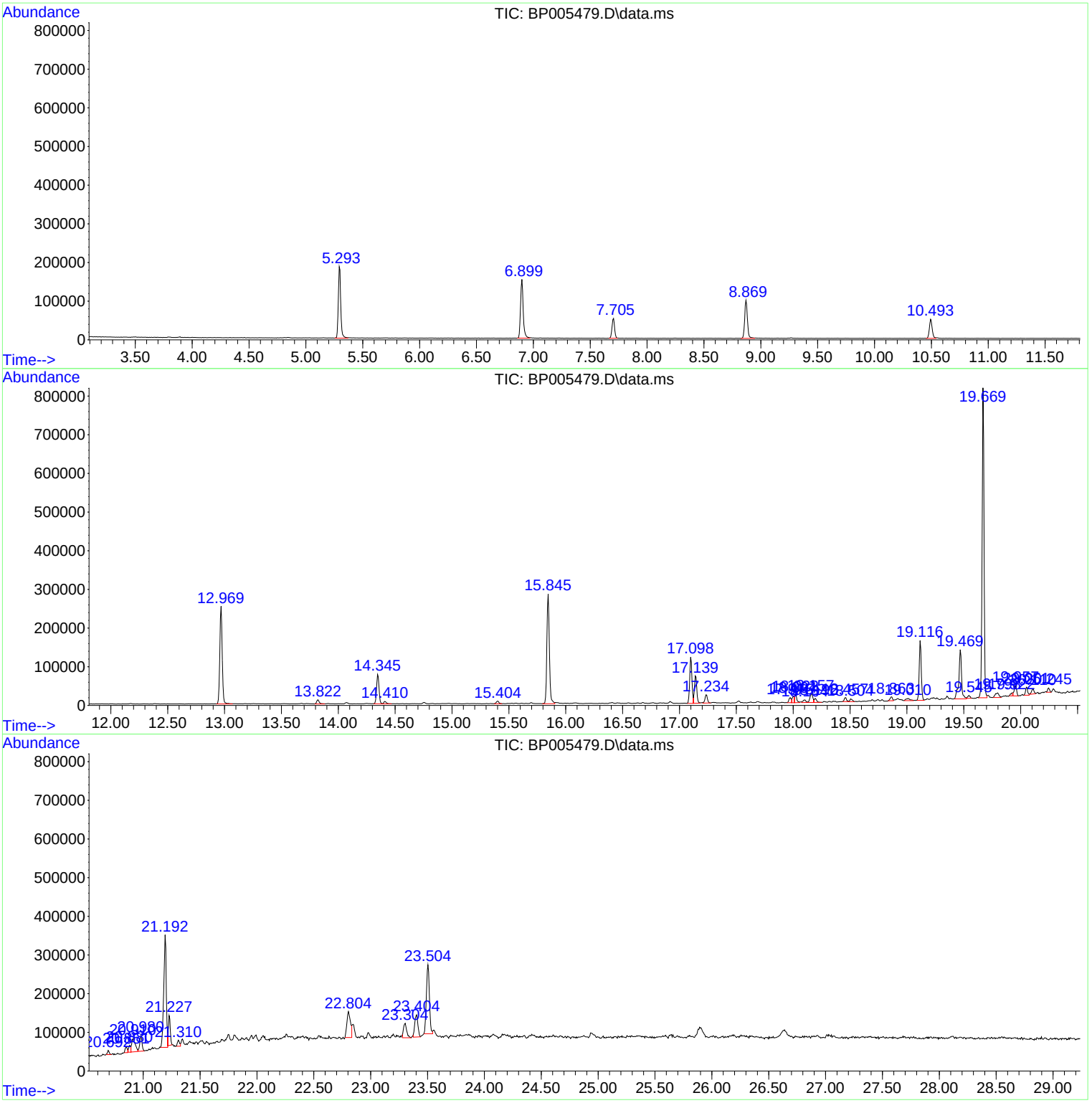
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

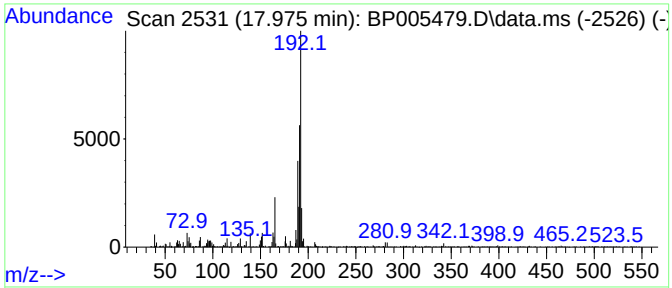
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

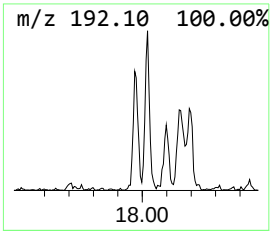
****

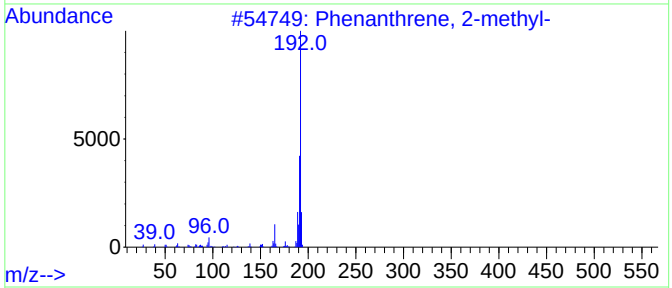
Peak Number 1 Phenanthrene, 2-methyl- Concentration Rank 6

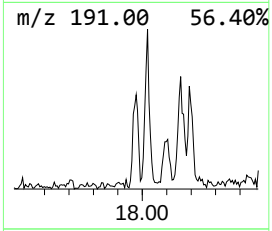
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.975	2.49 ng	20338	Phenanthrene-d10	17.098

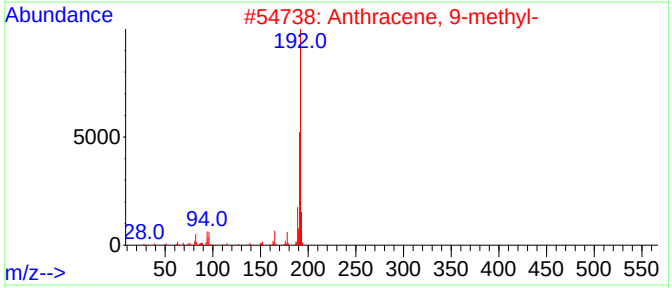
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	86
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	86
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	70

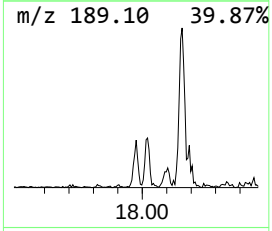


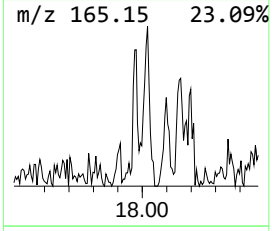


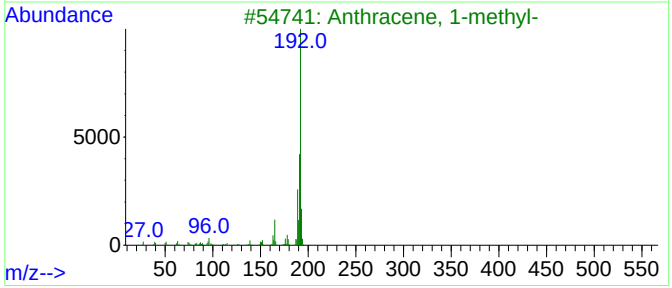


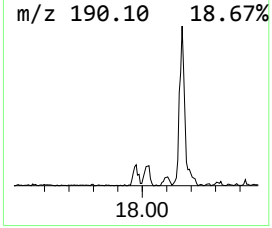












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

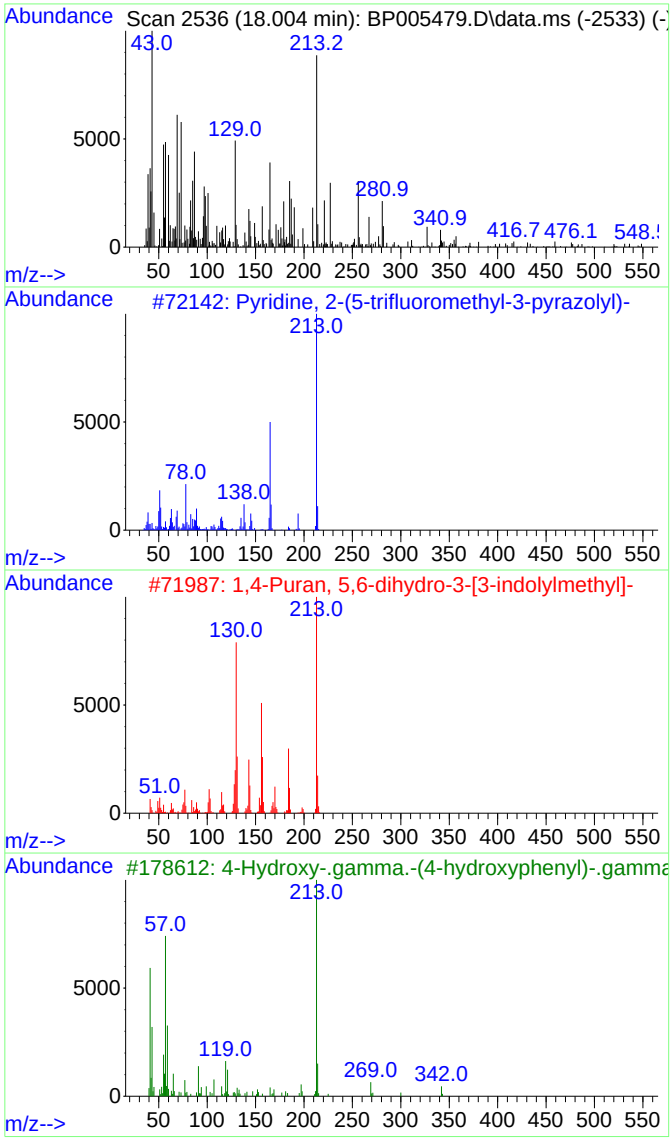
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

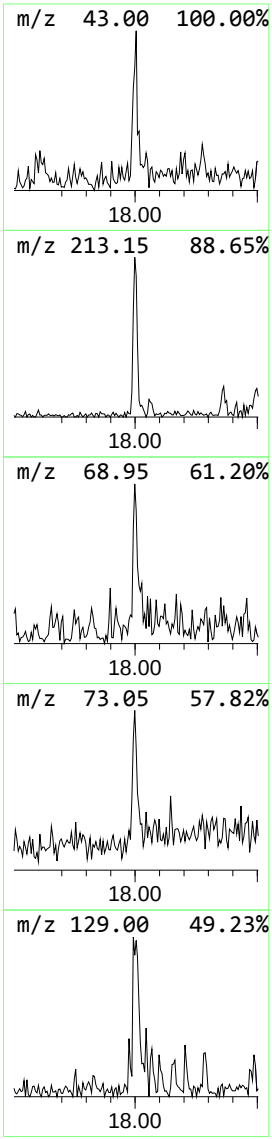
****

Peak Number 2 unknown18.004 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	2.54 ng	20784	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-71-8	27
2	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	18
3	4-Hydroxy-.gamma.-(4-hydroxyphen...	342	C21H26O4	138721-52-5	15
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	11
5	Malonic acid, 1,3-dithio-, bimol...	324	C10H12O4S4	021620-30-4	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
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Acq On : 10 May 2021 21:07
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Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

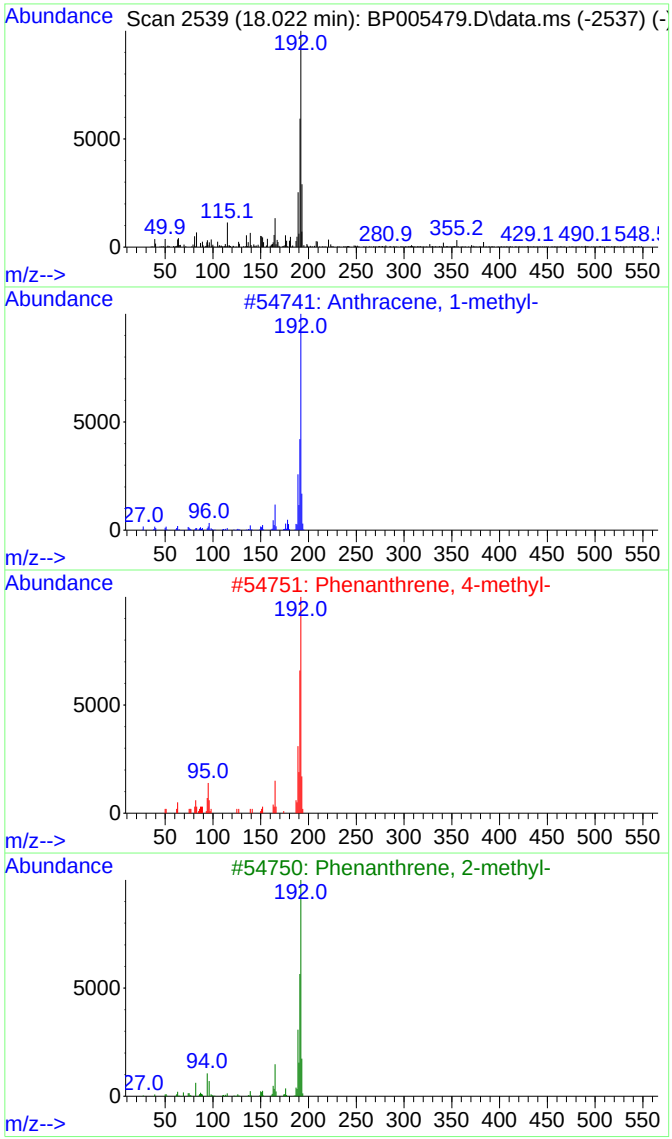
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

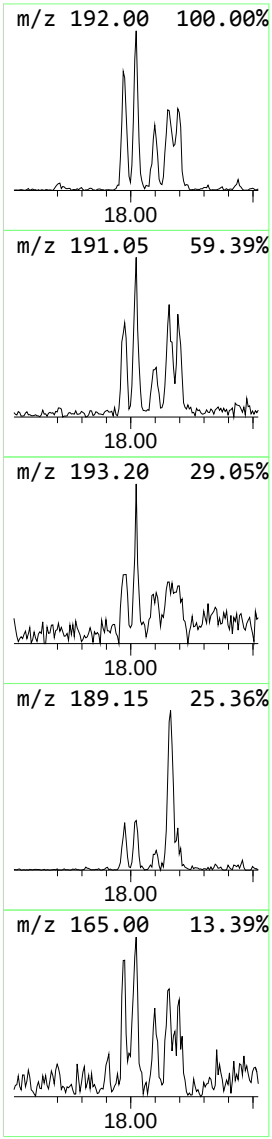
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	3.02 ng	24685	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	76
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
4	1-(Hydrazinocarbonylmethyl)-1-ph...	224	C9H12N4OS	013116-01-3	64
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BS-SP2

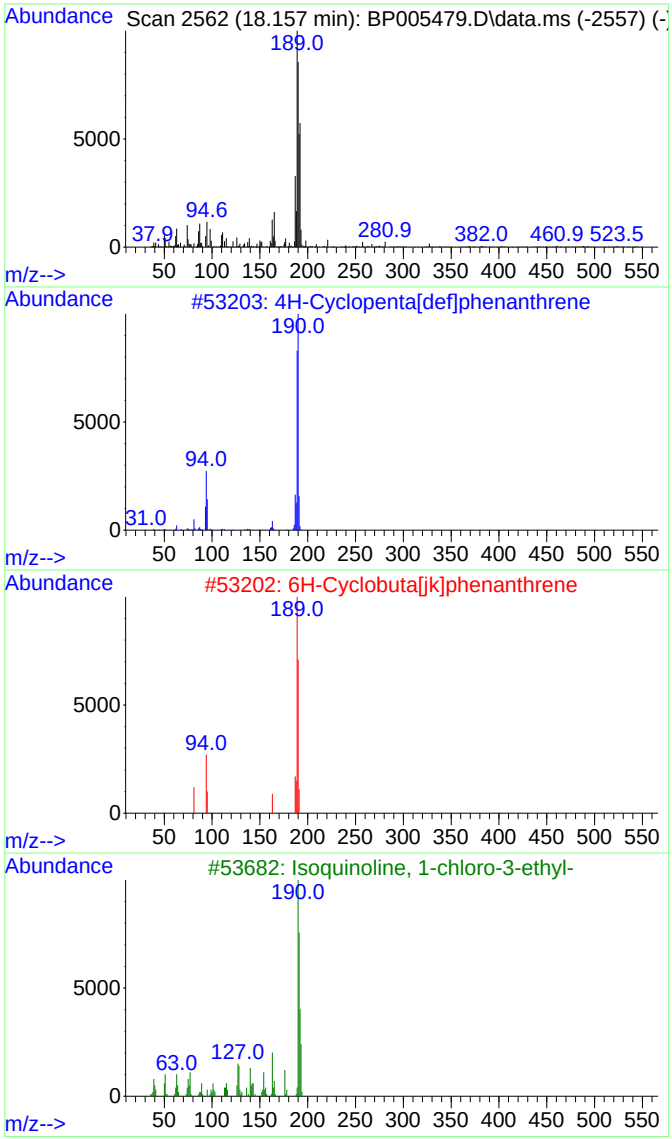
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

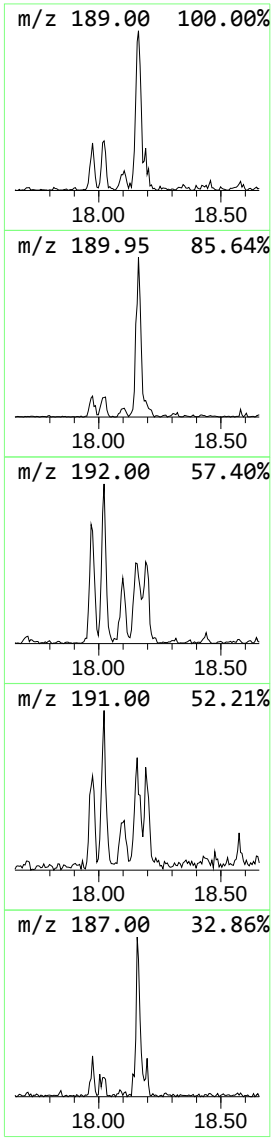
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	4.87 ng	39802	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	38
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	25





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Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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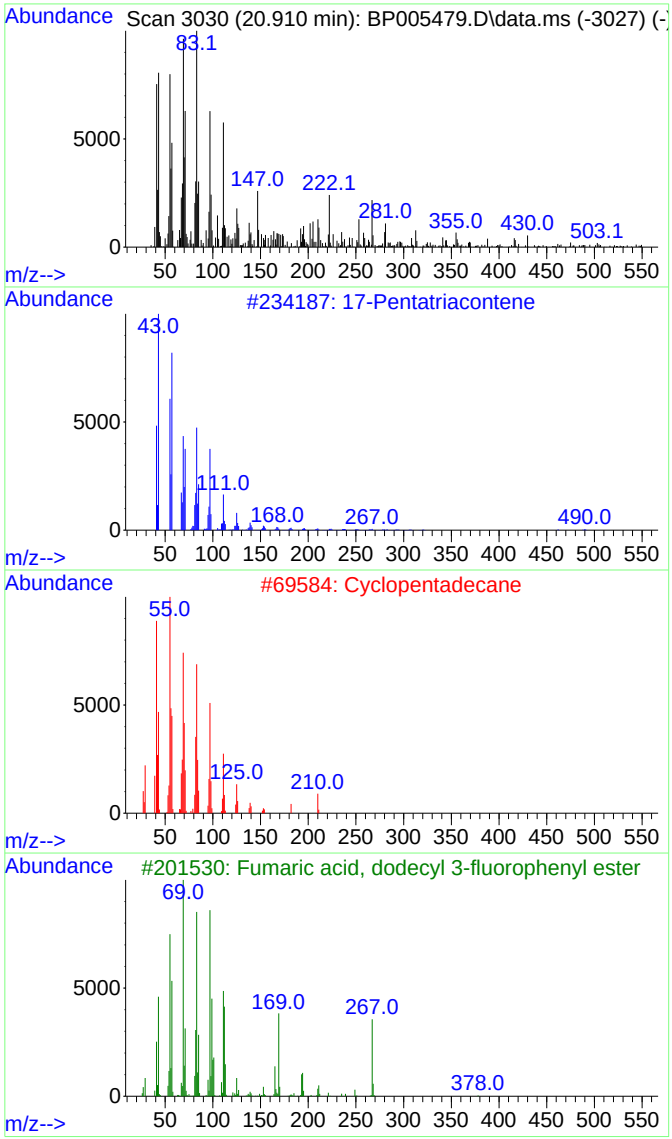
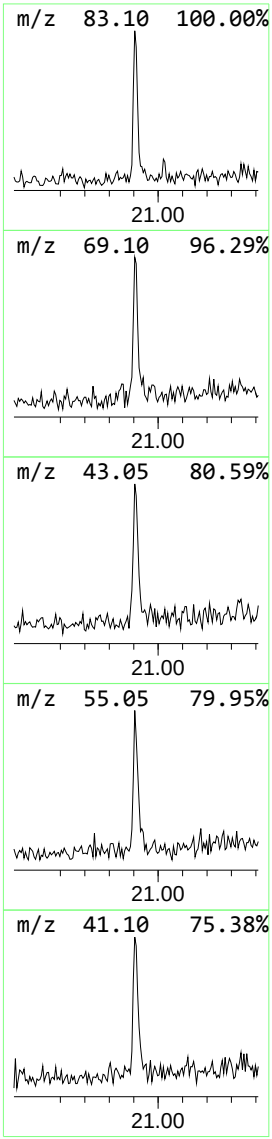
Peak Number 5 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.910	3.13 ng	71375	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	Cyclopentadecane	210	C15H30	000295-48-7	81
3	Fumaric acid, dodecyl 3-fluoroph...	378	C22H31FO4	1000345-20-9	81
4	1-Nonadecene	266	C19H38	018435-45-5	80
5	Cyclododecane	168	C12H24	000294-62-2	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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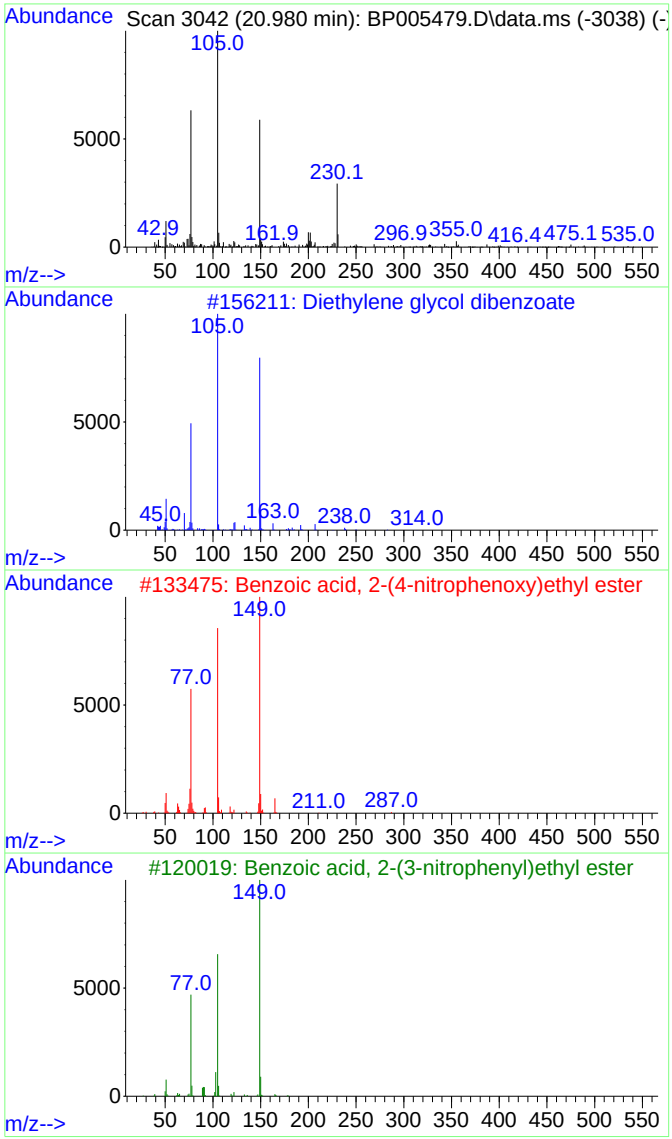
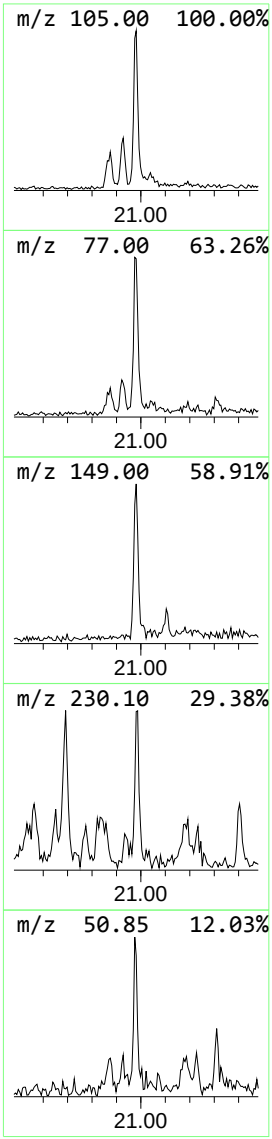
Peak Number 6 unknown20.980 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	2.35 ng	53552	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	45
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	45
3	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	45
4	Metomidate	230	C13H14N2O2	005377-20-8	38
5	Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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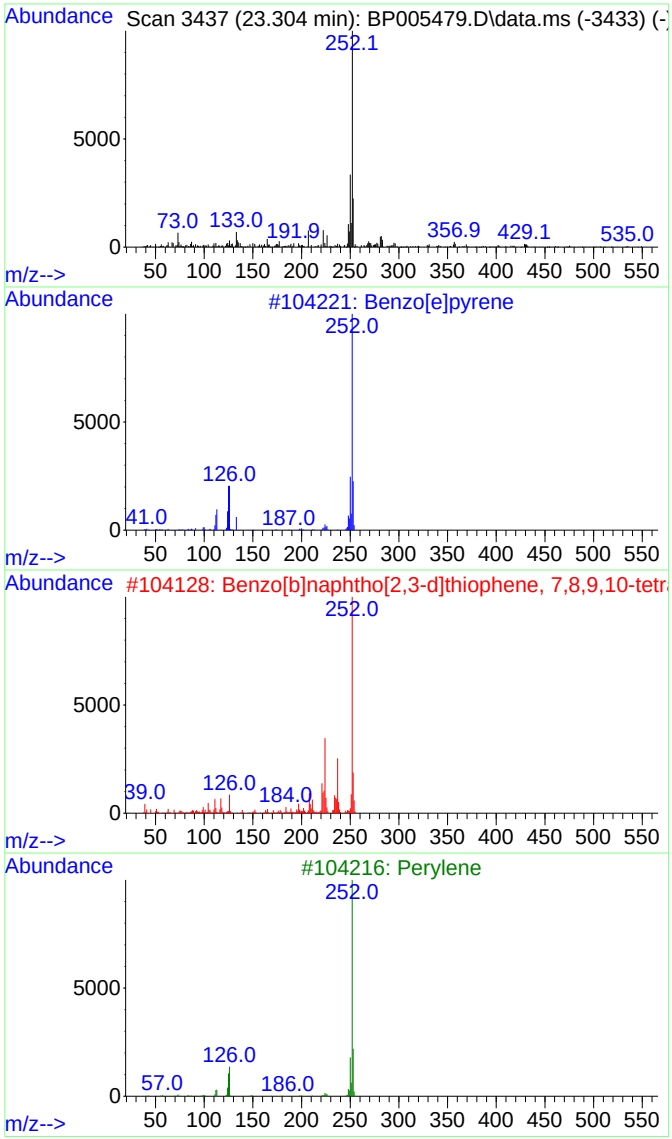
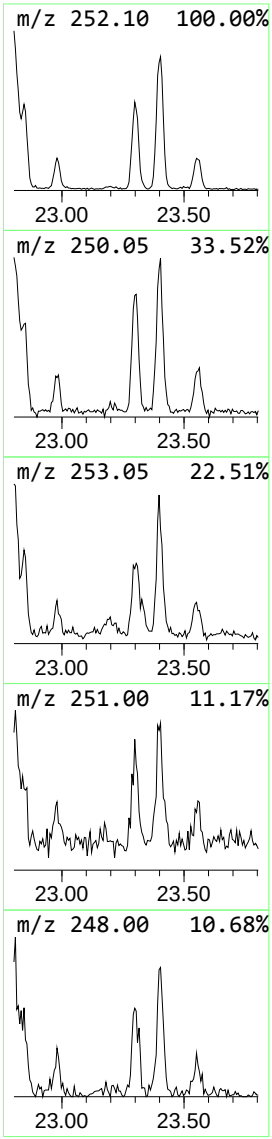
Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.304	4.23 ng	70053	Perylene-d12	23.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	62
2	Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-06-5	58
3	Perylene	252	C20H12	000198-55-0	53
4	2-[3-Methoxyphenyl]-4H-1-benzopy...	252	C16H12O3	053906-83-5	53
5	Benzo[a]pyrene	252	C20H12	000050-32-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051021\
Data File : BP005479.D
Acq On : 10 May 2021 21:07
Operator : CG/JU
Sample : M2310-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BS-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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
Phenanthrene, 2...	17.975	2.5	ng	20338	4	17.098	163618	20.0
unknown18.004	18.004	2.5	ng	20784	4	17.098	163618	20.0
Anthracene, 1-m...	18.022	3.0	ng	24685	4	17.098	163618	20.0
4H-Cyclopenta[d...	18.157	4.9	ng	39802	4	17.098	163618	20.0
17-Pentatriacon...	20.910	3.1	ng	71375	5	21.192	456359	20.0
unknown20.980	20.980	2.4	ng	53552	5	21.192	456359	20.0
Benzo[e]pyrene	23.304	4.2	ng	70053	6	23.504	331002	20.0