LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

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-BM040121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.922	3	6	22	rVB	700951	880726	22.19%	1.991%
2	5.269	399	405	422	rBV	1492279	2117103	53.34%	4.787%
3	6.845	666	673	689	rBV	1438435	2301942	58.00%	5.205%
4	7.669	807	813	820	rBV	364137	583771	14.71%	1.320%
5	8.822	998	1009	1019	rBV	882040	1478004	37.24%	3.342%
6	10.451	1279	1286	1292	rBV	453794	756206	19.05%	1.710%
7	12.933	1700	1708	1714	rBV	1888609	2785854	70.19%	6.299%
8	13.768	1842	1850	1860	rVB	123086	183695	4.63%	0.415%
9	14.027	1889	1894	1901	rBV	88639	151924	3.83%	0.344%
10	14.310	1935	1942	1948	rBV2	613504	903855	22.77%	2.044%
11	15.798	2188	2195	2203	rBV	1501227	2126574	53.58%	4.808%
12	16.786	2358	2363	2368	rBV2	22279	41574	1.05%	0.094%
13	17.051	2403	2408	2412	rBV	691741	1007701	25.39%	2.278%
14	17.098	2412	2416	2421	rVV	330995	477168	12.02%	1.079%
15	17.186	2423	2431	2437	rVV	218934	323043	8.14%	0.730%
16	17.574	2492	2497	2504	rVB3	31552	44661	1.13%	0.101%
17	17.927	2552	2557	2558	rBV	64318	72132	1.82%	0.163%
18	17.956	2558	2562	2572	rVV2	254315	508073	12.80%	1.149%
19	18.056	2574	2579	2583	rVV	61298	103553	2.61%	0.234%
20	18.121	2584	2590	2594	rVV2	144086	263825	6.65%	0.597%
21	18.156	2594	2596	2603	rVB	53354	67729	1.71%	0.153%
22	18.433	2638	2643	2647	rBV	75271	102662	2.59%	0.232%
23	18.845	2709	2713	2718	rBV3	53002	97074	2.45%	0.219%
24	18.986	2733	2737	2746	rVB	81887	131757	3.32%	0.298%
25	19.115	2752	2759	2766	rBV	1882715	2564241	64.61%	5.798%
26	19.262	2777	2784	2788	rBV2	179806	326327	8.22%	0.738%
27	19.356	2794	2800	2803	rBV	59462	91589	2.31%	0.207%
28	19.445	2810	2815	2816	rBV	227469	280694	7.07%	0.635%
29	19.474	2816	2820	2828	rVV	1965965	2623286	66.10%	5.931%
30	19.550	2828	2833	2839	rVB3	68075	120841	3.04%	0.273%
31	19.686	2846	2856	2860	rBV	3165609	3968826	100.00%	8.974%
32	19.797	2870	2875	2882	rBV4	98544	239475	6.03%	0.541%
33	19.933	2893	2898	2900	rBV3	85684	134886	3.40%	0.305%
34	19.968	2901	2904	2909	rVB	186169	265845	6.70%	0.601%
35	20.068	2917	2921	2925	rBV2	116538	146170	3.68%	0.330%
36	20.127	2925	2931	2936	rVV3	151522	252026	6.35%	0.570%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

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-BM040121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.209	2942	2945	2951	rBV3	27175	58628	1.48%	0.133%
38	20.268	2951	2955	2959	rBV	87922	109707	2.76%	0.248%
39	20.315	2959	2963	2967	rVV2	85058	117015	2.95%	0.265%
40	20.380	2970	2974	2979	rVB	247474	269889	6.80%	0.610%
41	20.715	3027	3031	3038	rVB2	91963	140520	3.54%	0.318%
42	20.880	3054	3059	3062	rBV3	106584	164013	4.13%	0.371%
43	20.921	3062	3066	3068	rVV	121456	139435	3.51%	0.315%
44	20.956	3068	3072	3077	rVV2	493601	634882	16.00%	1.436%
45	21.221	3112	3117	3122	rBV2	1488544	2862455	72.12%	6.472%
46	21.268	3122	3125	3133	rVB	878335	1148502	28.94%	2.597%
47	21.386	3142	3145	3150	rBV2	147170	229633	5.79%	0.519%
48	21.433	3150	3153	3157	rVV	108283	136077	3.43%	0.308%
49	21.544	3167	3172	3177	rBV2	105336	199880	5.04%	0.452%
50	21.774	3209	3211	3216	rVB	146153	171765	4.33%	0.388%
51	21.827	3217	3220	3227	rVB	112431	161265	4.06%	0.365%
52	22.780	3376	3382	3387	rBV	930517	2104573	53.03%	4.759%
53	22.950	3406	3411	3417	rVB	204392	335274	8.45%	0.758%
54	23.250	3457	3462	3471	rVB	573130	1083611	27.30%	2.450%
55	23.344	3472	3478	3485	rVV	1003215	1737802	43.79%	3.929%
56	23.438	3488	3494	3499	rVV2	601889	1229380	30.98%	2.780%
57	23.485	3499	3502	3511	rVB	291085	538899	13.58%	1.218%
58	25.656	3863	3871	3882	rVB2	450632	1210075	30.49%	2.736%
59	26.332	3980	3986	3997	rVB	336286	919087	23.16%	2.078%

Sum of corrected areas: 44227179

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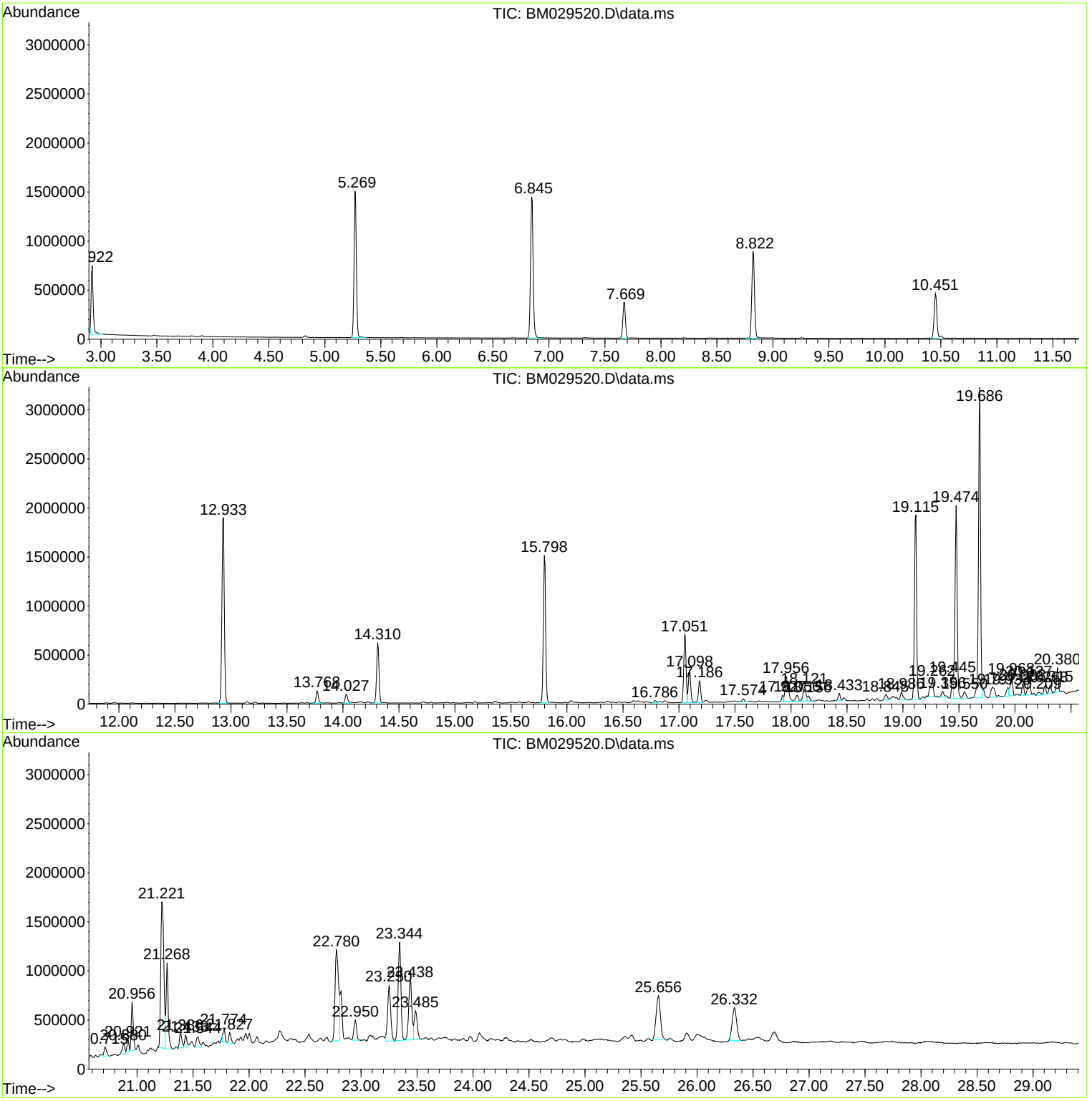
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
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Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

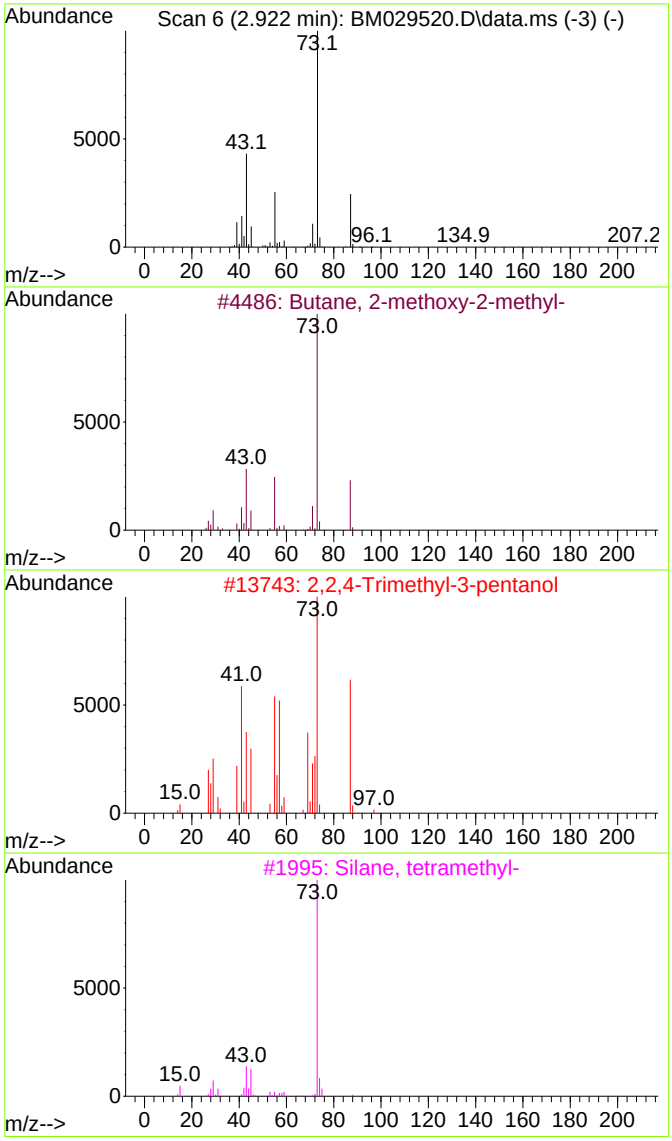
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

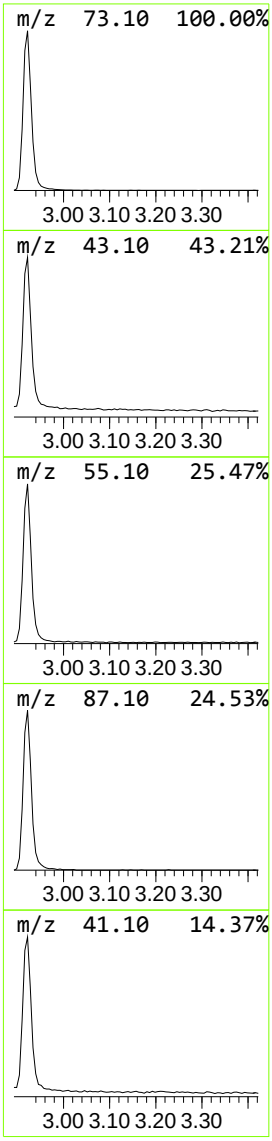
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	30.17 ng	880726	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

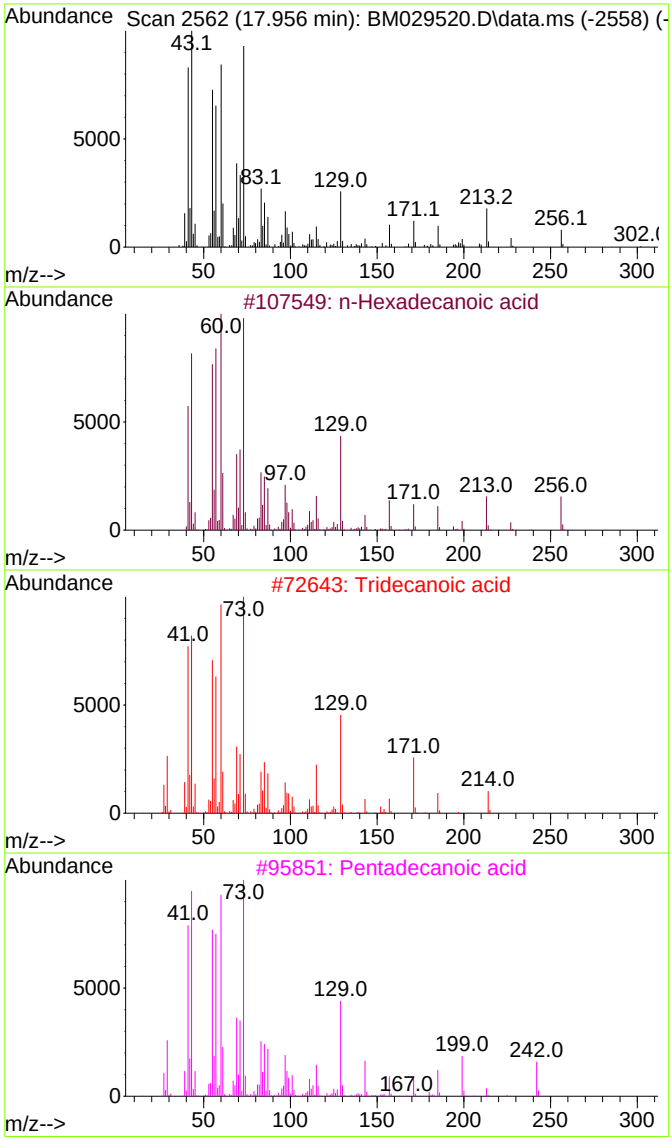
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

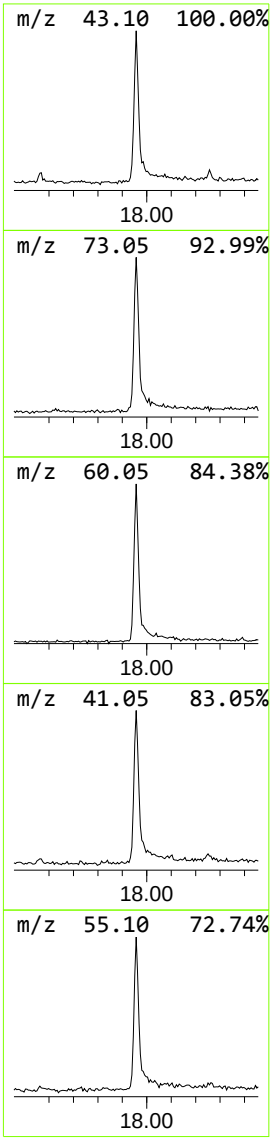
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.956	10.08 ng	508073	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

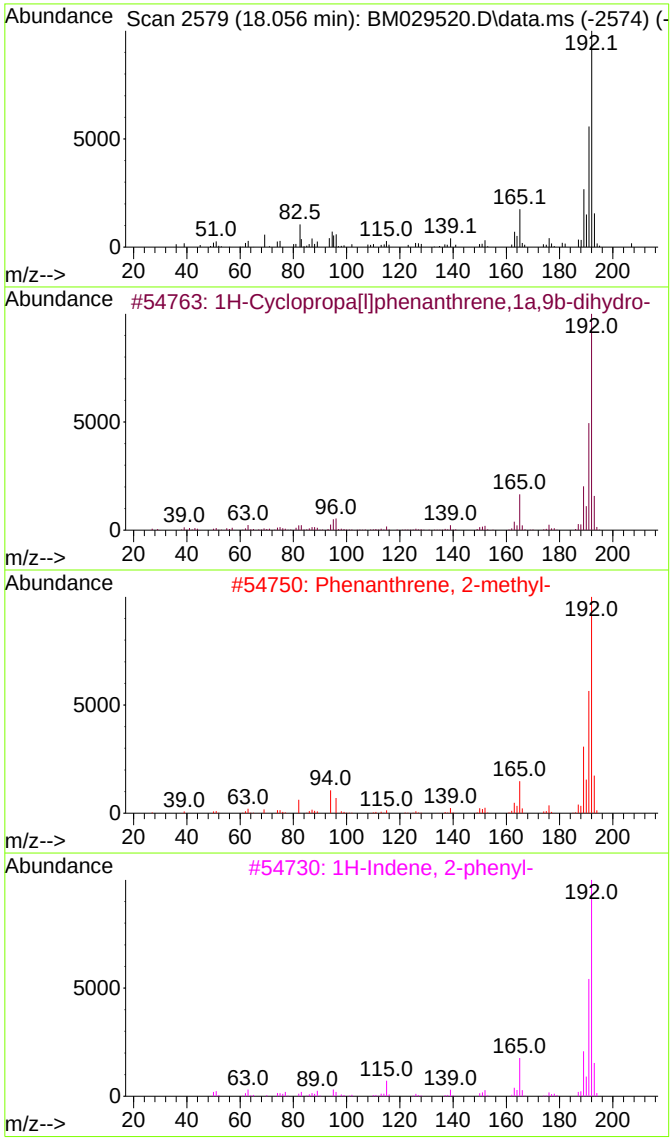
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

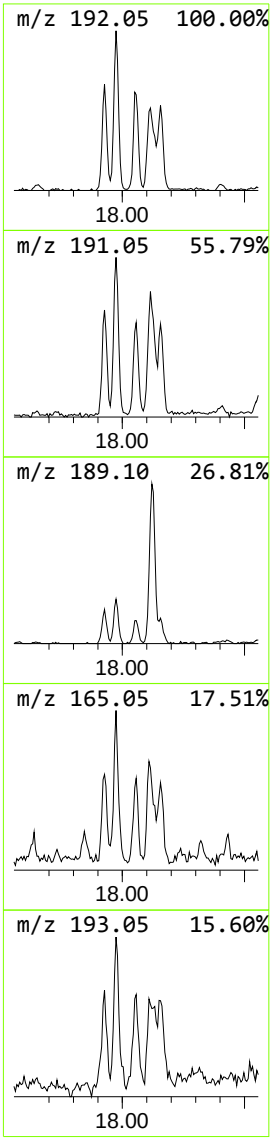
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1H-Cyclopropa[l]phenanthren... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	2.06 ng	103553	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

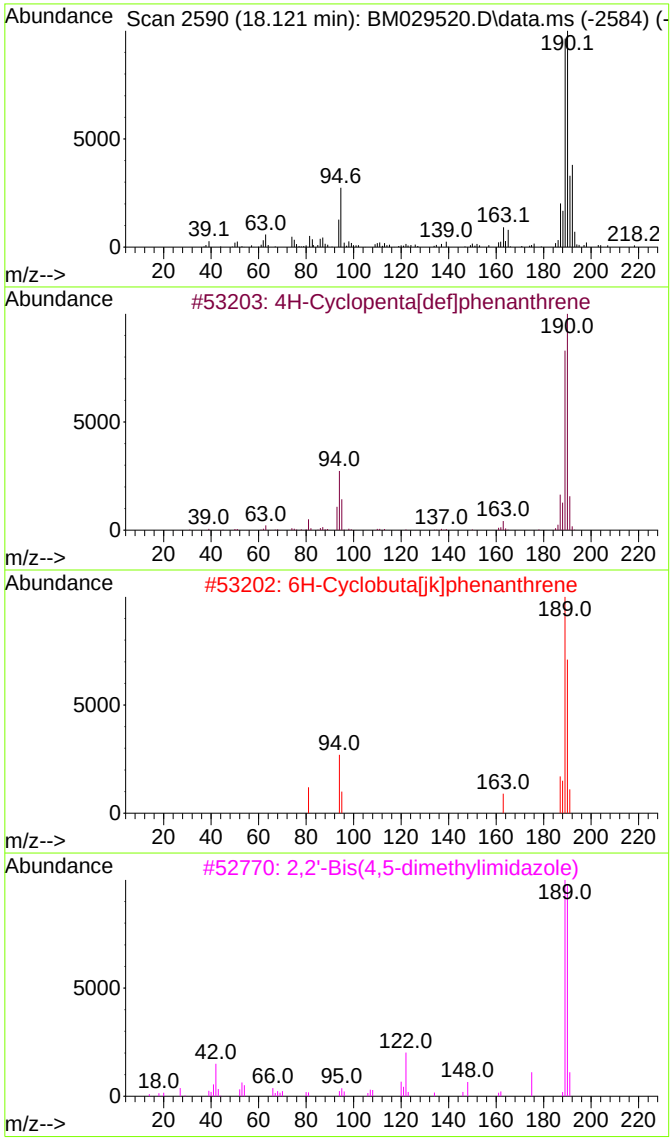
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

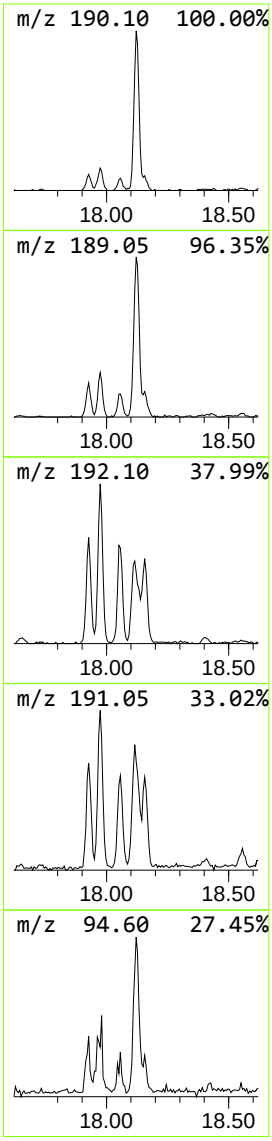
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	5.24 ng	263825	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
4	4-Isothiazolecarbonitrile, 5-chl...	190	C5H3ClN2S2	054798-93-5	12
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	10





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Data File : BM029520.D
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

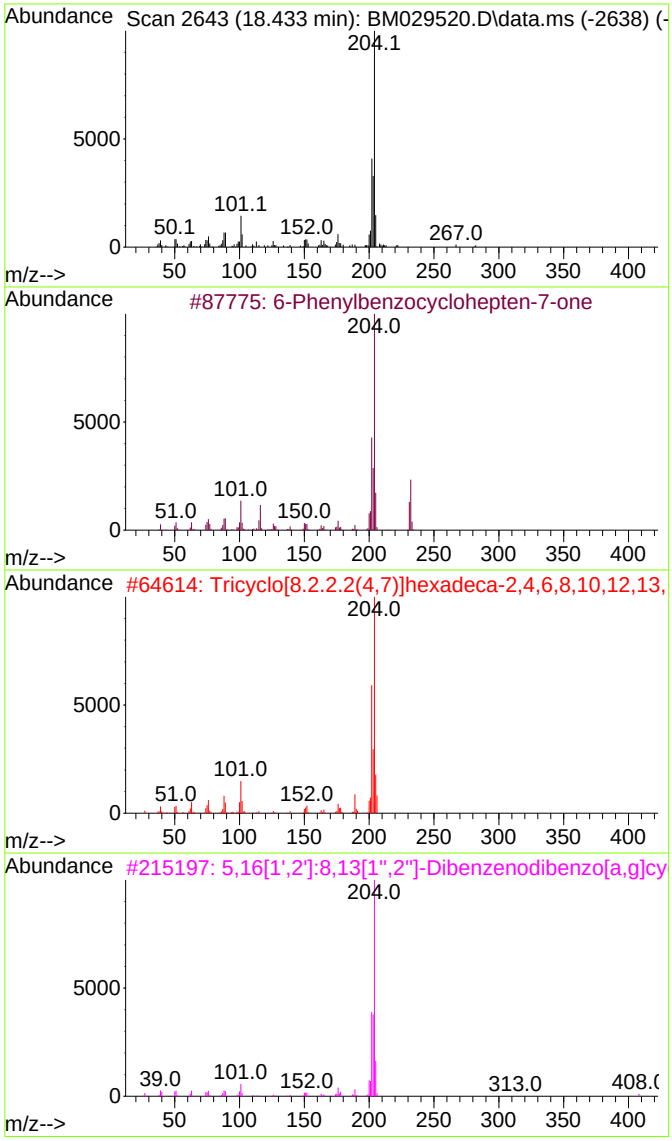
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

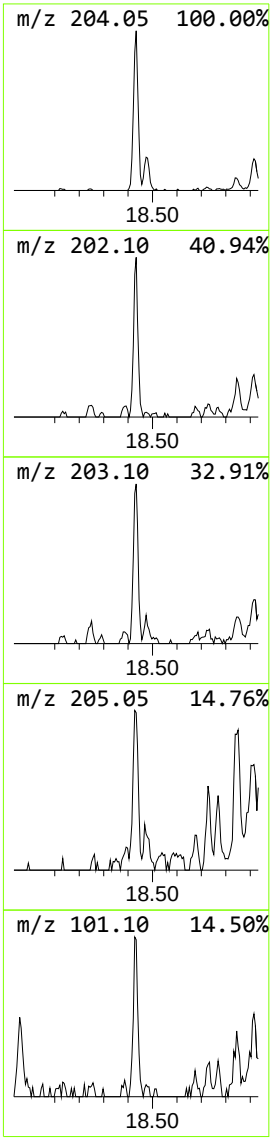
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 6-Phenylbenzocyclohepten-7-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	2.04 ng	102662	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	90
2	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	89
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	83
4	9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	78
5	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	70





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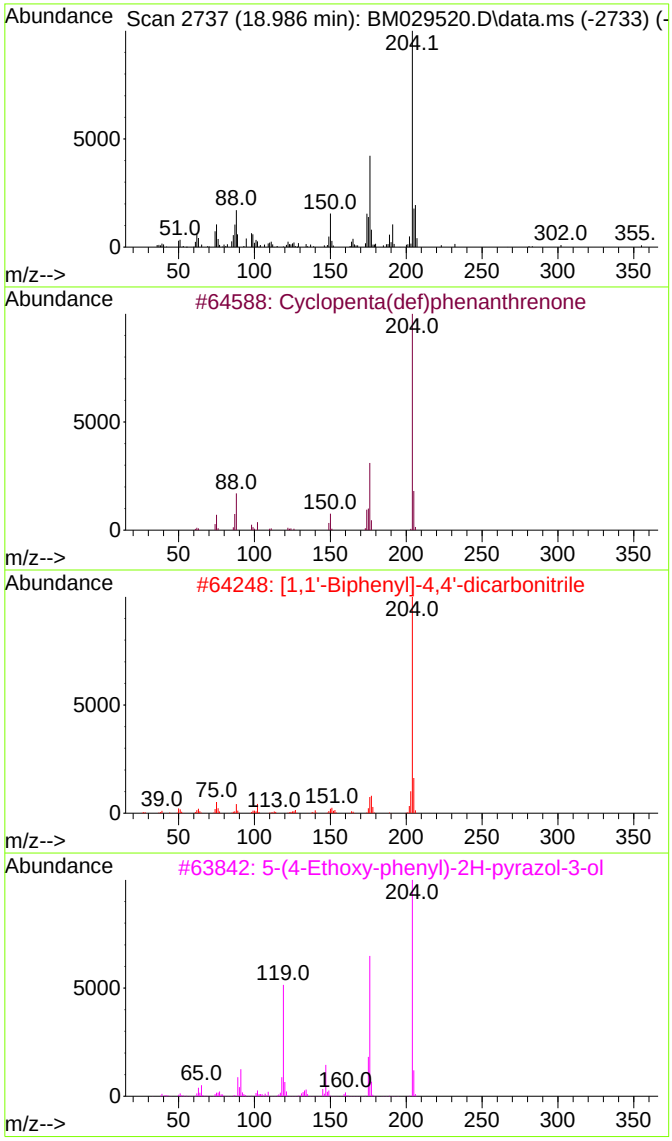
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

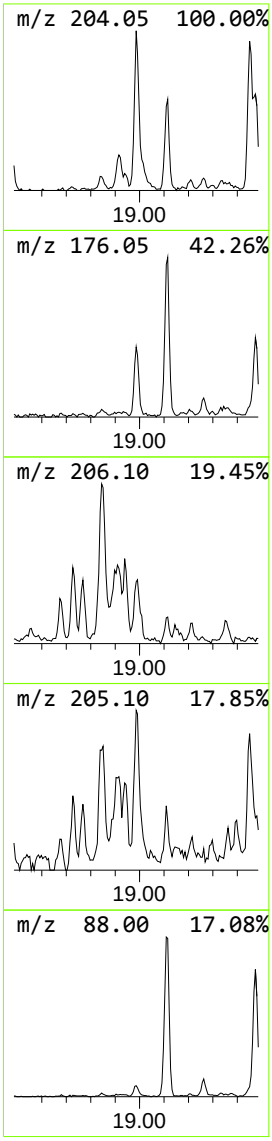
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	2.62 ng	131757	Phenanthrene-d10	17.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	87
2	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	52
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	50
4	Pyrene, 4,5-dihydro-	204	C16H12	006628-98-4	46
5	N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1000296-34-3	40





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Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

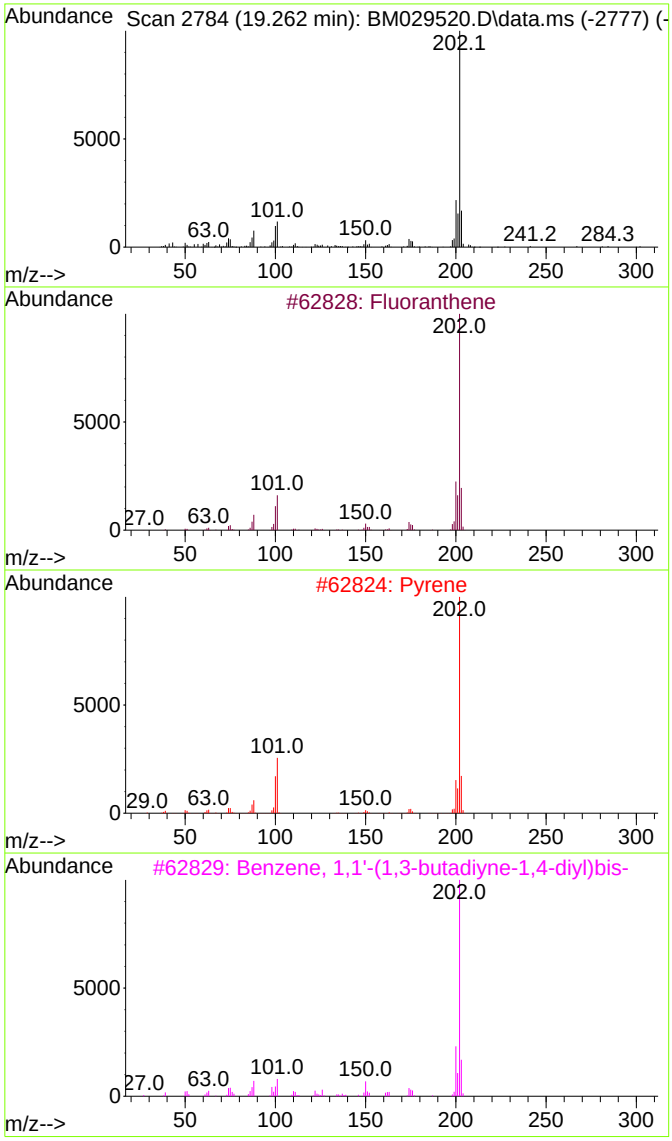
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

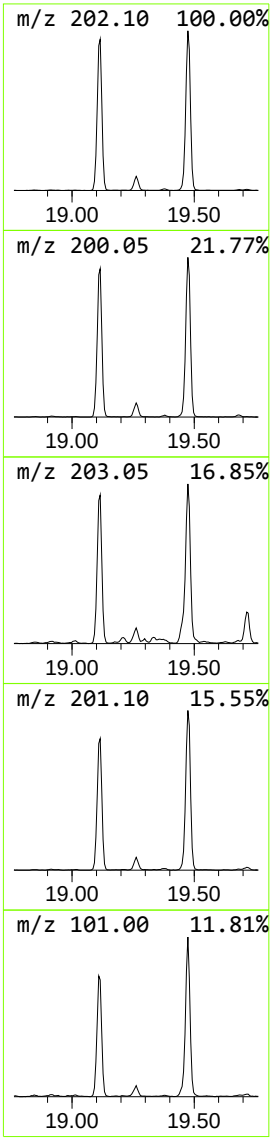
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	2.28 ng	326327	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	98
2	Pyrene	202	C16H10	000129-00-0	89
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	81
4	l-Leucine, N-methyl-N-(2-methoxy...	499	C29H57NO5	1000328-55-2	47
5	l-Leucine, N-methyl-N-(2-methoxy...	471	C27H53NO5	1000328-55-0	47





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Data File : BM029520.D
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Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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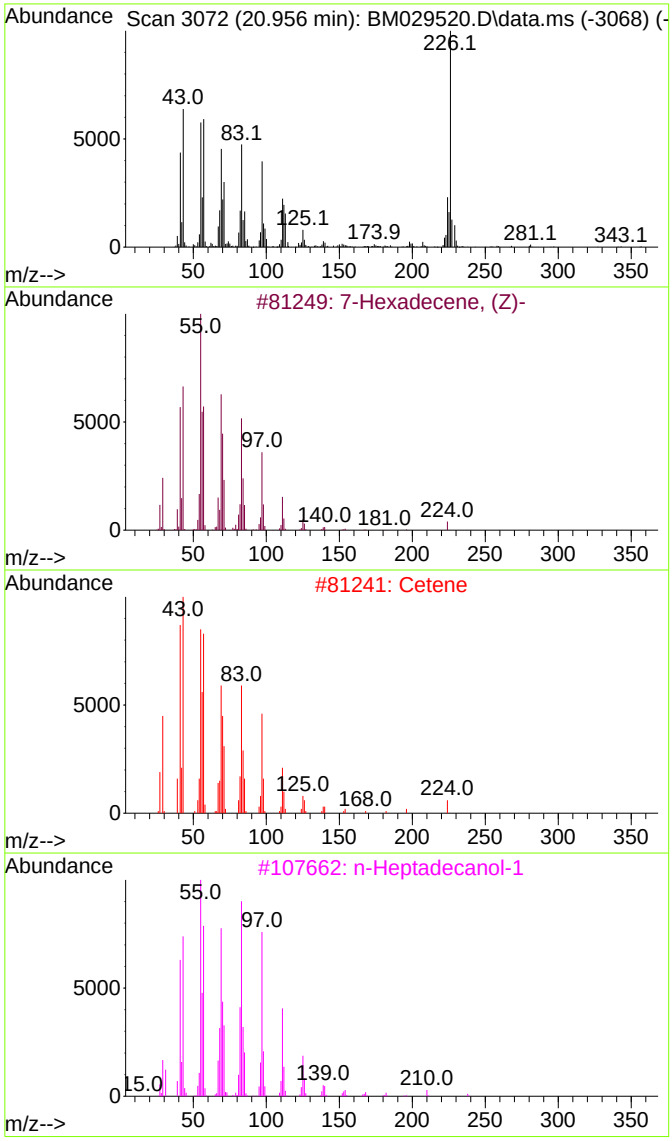
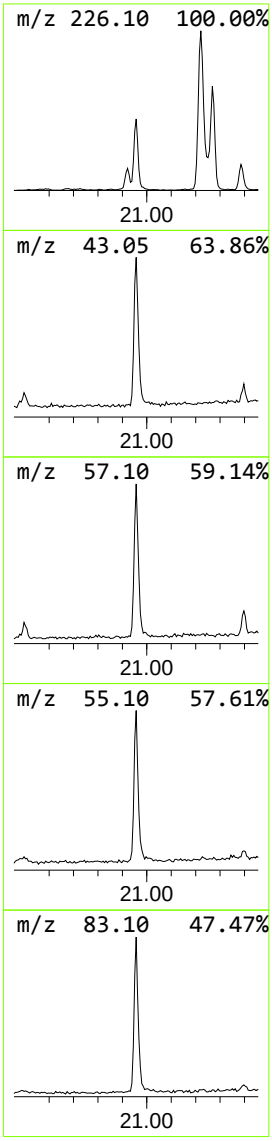
Peak Number 8 unknown20.956 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.956	4.44 ng	634882	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	45
2	Cetene	224	C16H32	000629-73-2	43
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	42
4	Benzo[ghi]fluoranthene	226	C18H10	000203-12-3	41
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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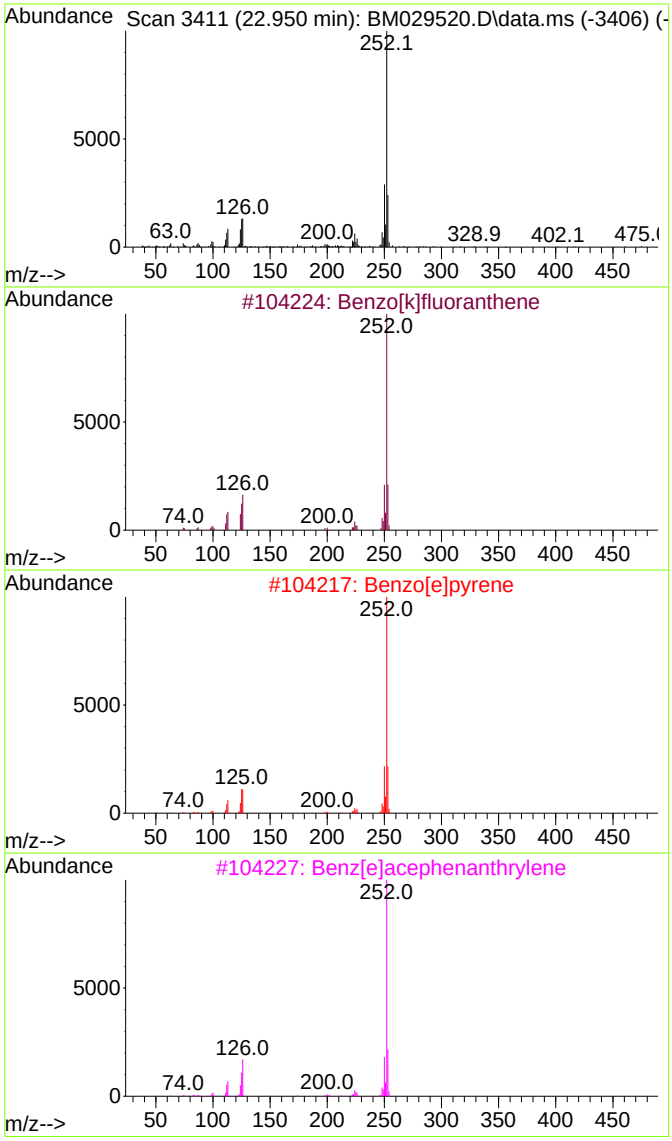
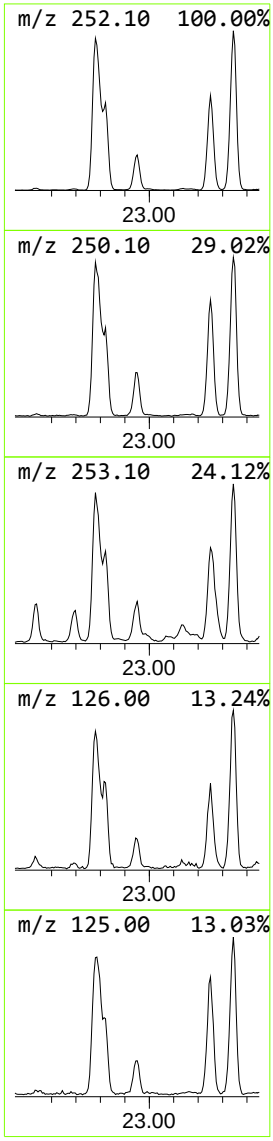
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.950	5.45 ng	335274	Perylene-d12	23.438

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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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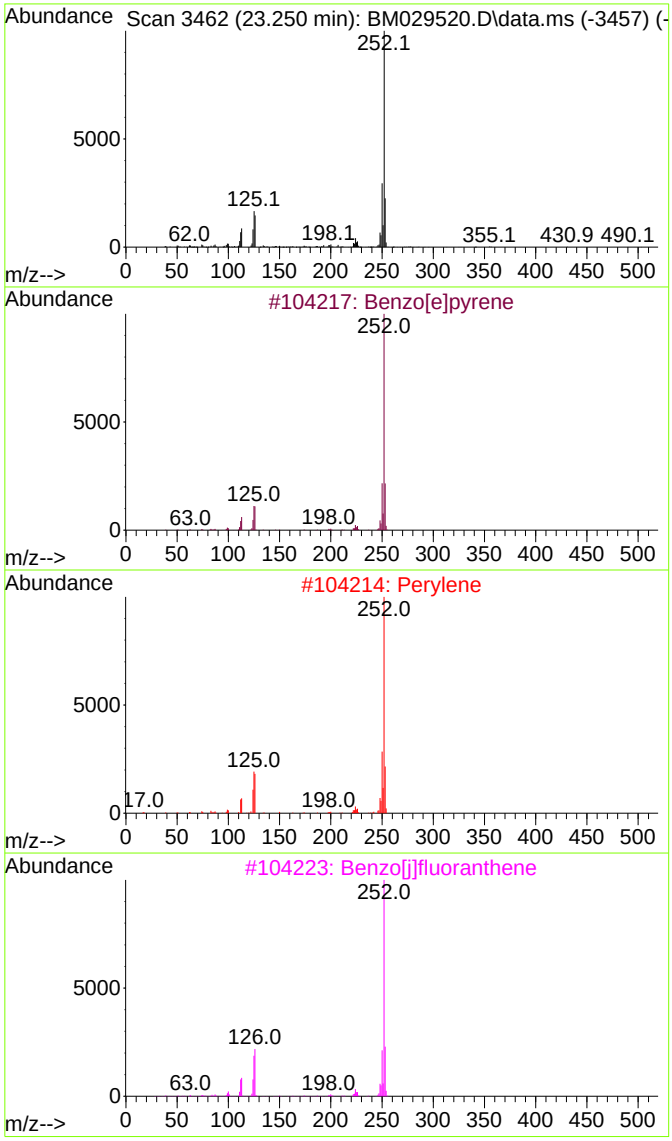
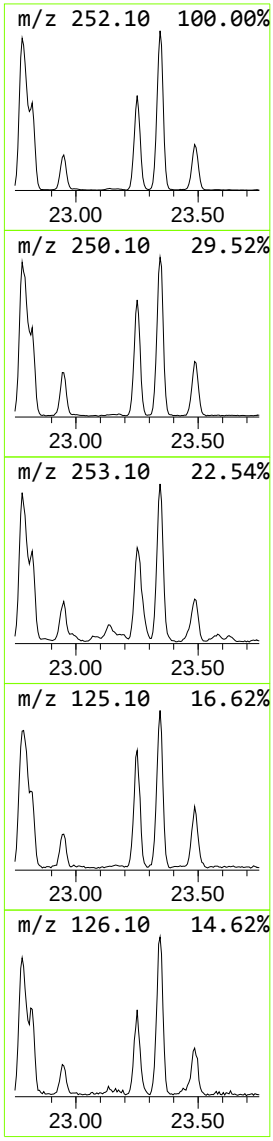
Peak Number 10 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.250	17.63 ng	1083610	Perylene-d12	23.438

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	99
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029520.D
Acq On : 16 Apr 2021 14:04
Operator : CG/JU
Sample : M1947-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FS-SB19B(19-20)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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
Butane, 2-metho...	2.922	30.2	ng	880726	1	7.675	583771	20.0
n-Hexadecanoic ...	17.956	10.1	ng	508073	4	17.051	1007700	20.0
1H-Cyclopropa[l...	18.056	2.1	ng	103553	4	17.051	1007700	20.0
4H-Cyclopenta[d...	18.121	5.2	ng	263825	4	17.051	1007700	20.0
6-Phenylbenzocy...	18.433	2.0	ng	102662	4	17.051	1007700	20.0
Cyclopenta(def)...	18.986	2.6	ng	131757	4	17.051	1007700	20.0
Benzene, 1,1'-(...	19.262	2.3	ng	326327	5	21.233	2862460	20.0
unknown20.956	20.956	4.4	ng	634882	5	21.233	2862460	20.0
Benzo[e]pyrene	22.950	5.5	ng	335274	6	23.438	1229380	20.0
Perylene	23.250	17.6	ng	1083610	6	23.438	1229380	20.0