LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

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-BP011221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.399	370	376	397	rBV	3015324	4573488	36.94%	5.639%
2	6.987	637	646	665	rBV	2827196	4838129	39.07%	5.965%
3	7.810	778	786	795	rBV	725784	1168624	9.44%	1.441%
4	8.969	975	983	998	rBV	1830513	3071060	24.80%	3.786%
5	10.604	1253	1261	1267	rBV	939958	1686160	13.62%	2.079%
6	10.657	1267	1270	1281	rVB	200533	315951	2.55%	0.390%
7	12.275	1536	1545	1553	rBV	224382	377976	3.05%	0.466%
8	12.493	1574	1582	1591	rVB	134639	227921	1.84%	0.281%
9	13.075	1674	1681	1695	rBV	5229464	8017752	64.75%	9.885%
10	13.292	1712	1718	1725	rBV2	99159	162372	1.31%	0.200%
11	13.781	1794	1801	1806	rBV	90045	173854	1.40%	0.214%
12	13.910	1818	1823	1828	rBV	113915	163576	1.32%	0.202%
13	14.463	1907	1917	1922	rBV	1602646	2401897	19.40%	2.961%
14	14.528	1922	1928	1935	rVB	852525	1345724	10.87%	1.659%
15	14.863	1979	1985	1993	rVB	368058	552153	4.46%	0.681%
16	15.516	2090	2096	2107	rVB	639546	926095	7.48%	1.142%
17	15.810	2142	2146	2154	rVB	127015	199850	1.61%	0.246%
18	15.957	2164	2171	2180	rBV	4666806	6886714	55.62%	8.490%
19	16.522	2262	2267	2272	rVB2	76939	128235	1.04%	0.158%
20	16.951	2335	2340	2348	rBV3	50861	135955	1.10%	0.168%
21	17.039	2350	2355	2364	rVB	143351	229783	1.86%	0.283%
22	17.222	2380	2386	2390	rBV	1932886	2980577	24.07%	3.675%
23	17.263	2390	2393	2401	rVV	2290994	3237686	26.15%	3.992%
24	17.357	2404	2409	2414	rVB	173364	279797	2.26%	0.345%
25	18.092	2529	2534	2539	rBV	195528	383973	3.10%	0.473%
26	18.139	2539	2542	2546	rVB	255972	331168	2.67%	0.408%
27	18.286	2560	2567	2571	rVV2	454602	759555	6.13%	0.936%
28	18.580	2612	2617	2629	rVB2	134950	325131	2.63%	0.401%
29	18.851	2659	2663	2668	rVB	516872	619372	5.00%	0.764%
30	18.939	2674	2678	2681	rBV	134848	161437	1.30%	0.199%
31	19.239	2723	2729	2735	rBV	2740586	3457960	27.93%	4.263%
32	19.469	2764	2768	2775	rBV2	177457	253865	2.05%	0.313%
33	19.563	2779	2784	2785	rVV	474441	597797	4.83%	0.737%
34	19.592	2785	2789	2797	rVV	1680410	2385925	19.27%	2.942%
35	19.786	2815	2822	2828	rBV	9876832	12382421	100.00%	15.266%
36	19.910	2838	2843	2844	rBV	81148	135590	1.10%	0.167%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

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-BP011221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.074	2861	2871	2876	rVB	289955	512532	4.14%	0.632%
38	20.169	2883	2887	2892	rBV	251445	369925	2.99%	0.456%
39	20.451	2932	2935	2940	rVB	146365	190159	1.54%	0.234%
40	20.657	2966	2970	2974	rBV	619015	705121	5.69%	0.869%
41	20.704	2975	2978	2985	rVB	132236	174312	1.41%	0.215%
42	20.986	3020	3026	3029	rBV2	183885	459349	3.71%	0.566%
43	21.033	3029	3034	3040	rVV3	636938	1354361	10.94%	1.670%
44	21.086	3040	3043	3050	rVB	660445	868162	7.01%	1.070%
45	21.221	3062	3066	3072	rVB	1094513	1227296	9.91%	1.513%
46	21.316	3075	3082	3086	rVV2	2958345	4477653	36.16%	5.520%
47	21.351	3086	3088	3098	rVB	468527	552743	4.46%	0.681%
48	21.474	3105	3109	3116	rVB	109294	161205	1.30%	0.199%
49	22.186	3227	3230	3236	rVB3	126153	166429	1.34%	0.205%
50	22.951	3356	3360	3366	rBV	186721	387082	3.13%	0.477%
51	23.668	3475	3482	3490	rBV2	1822179	3629555	29.31%	4.475%

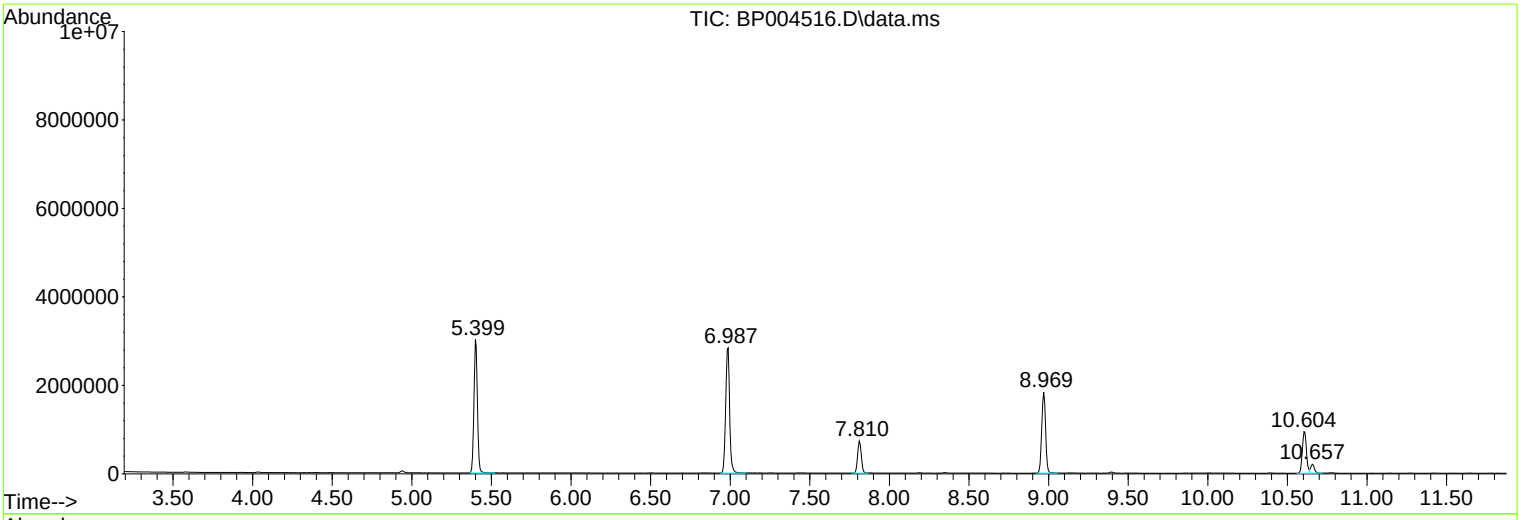
Sum of corrected areas: 81111407

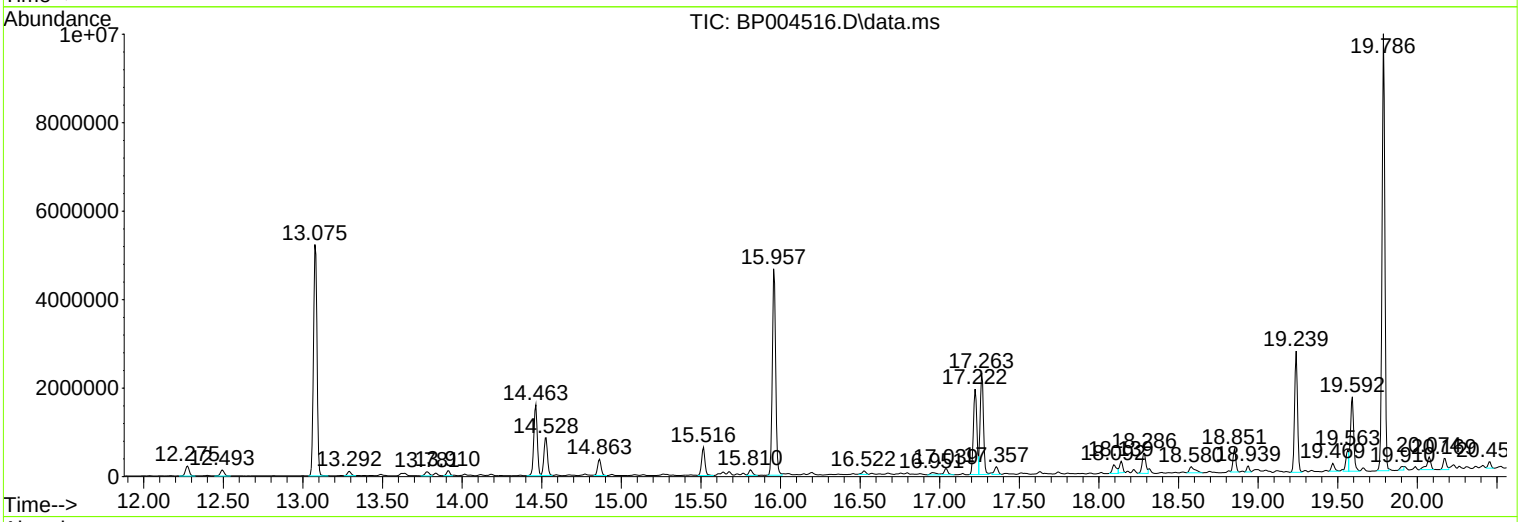
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

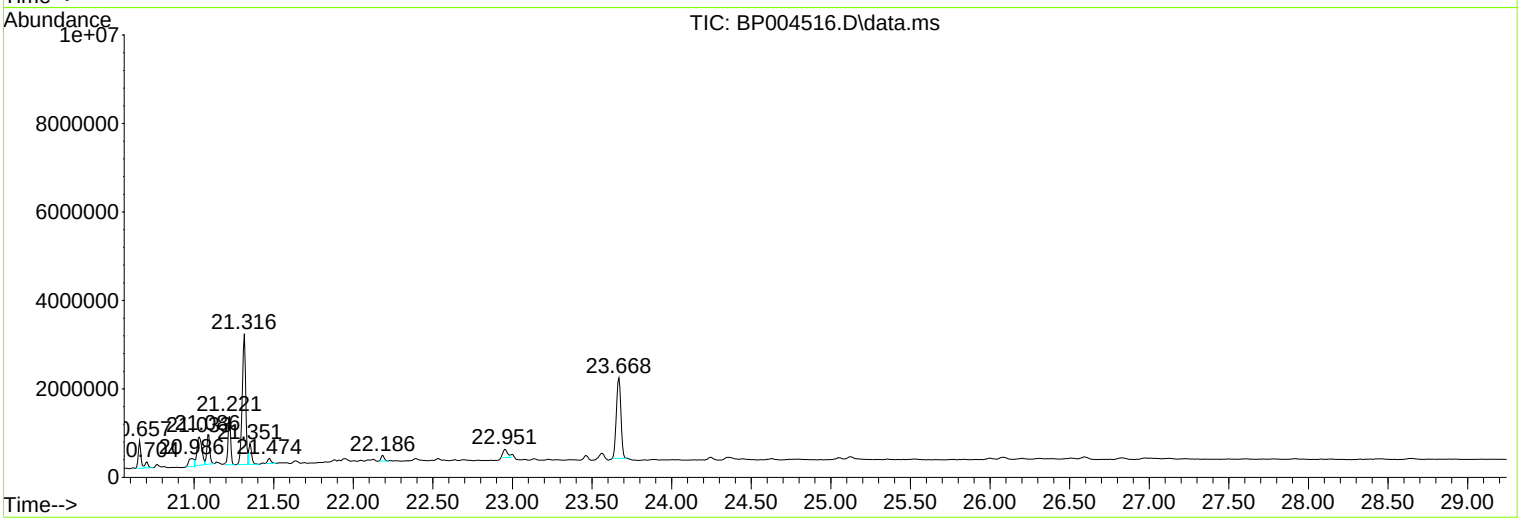
Instrument :
BNA_P
ClientSampleId :
72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.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\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

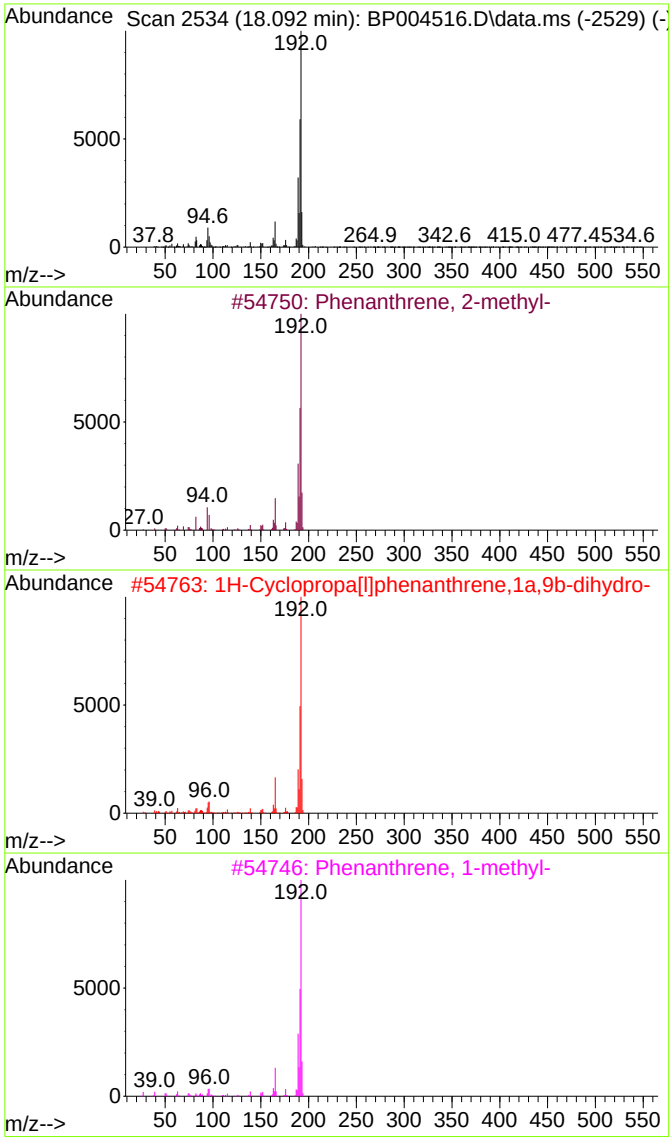
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

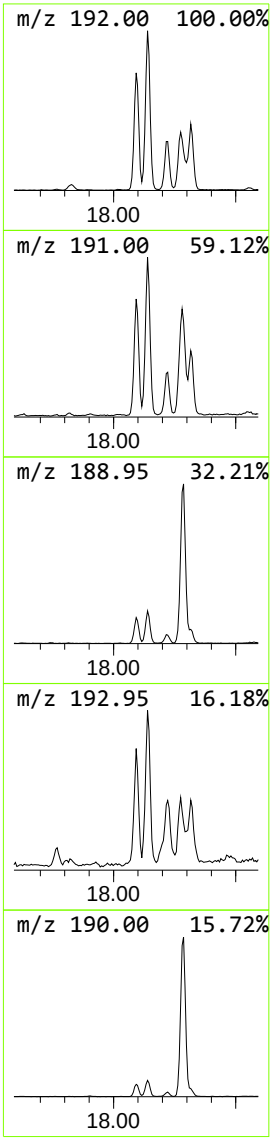
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	2.58 ng	383973	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

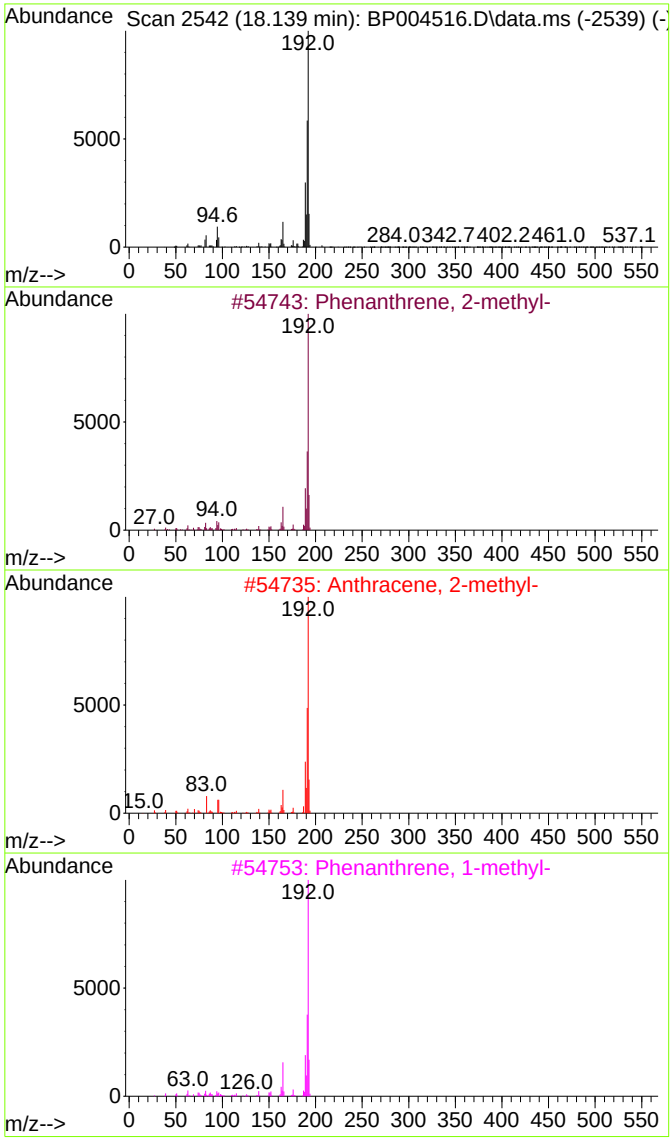
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

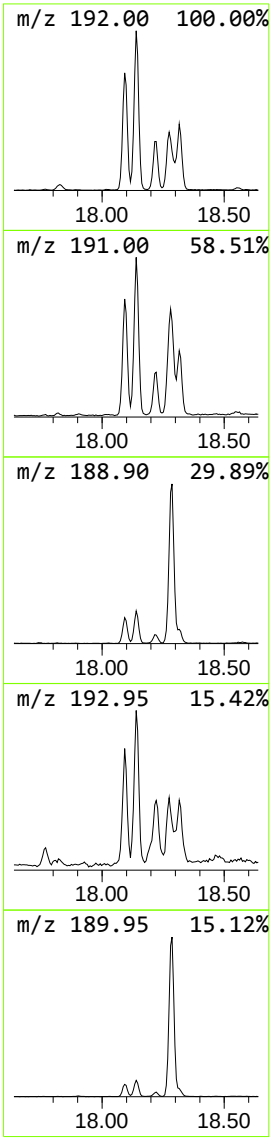
****

Peak Number 2 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	2.22 ng	331168	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

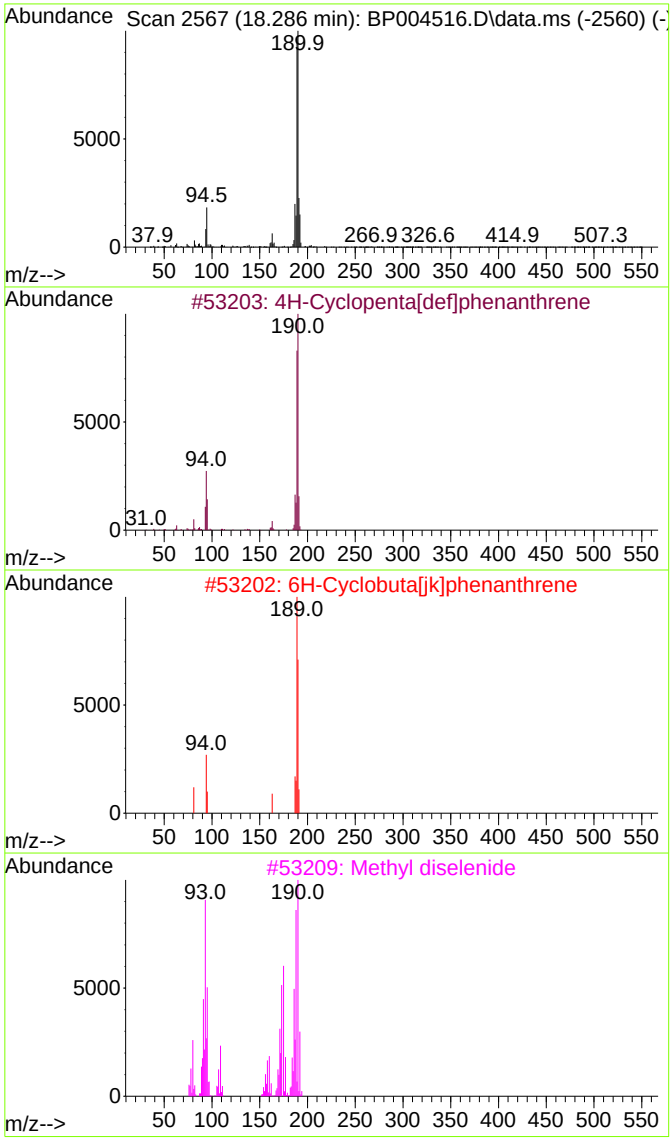
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

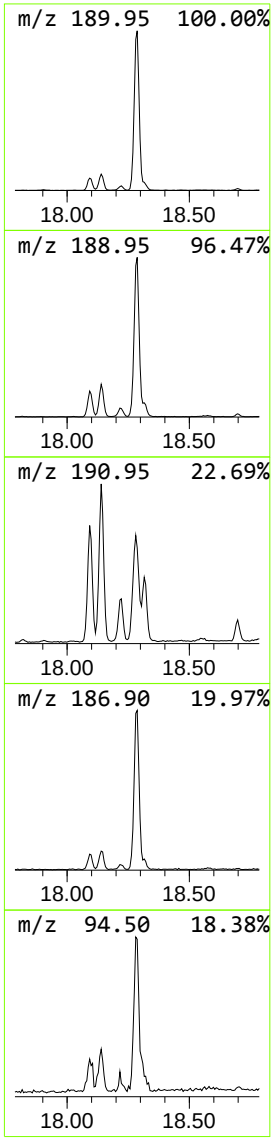
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	5.10 ng	759555	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	78
3	Methyl diselenide	190	C2H6Se2	007101-31-7	55
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	53
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

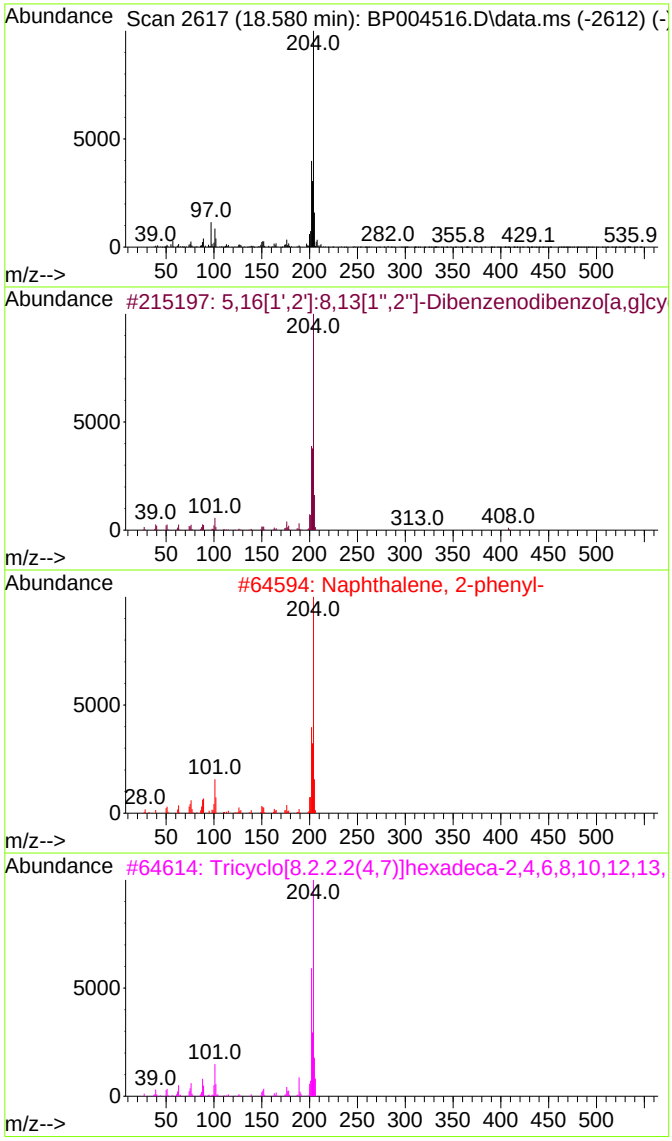
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

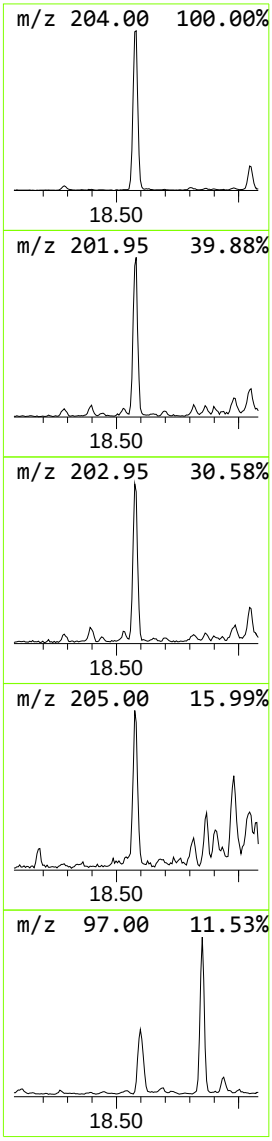
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.580	2.18 ng	325131	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	87
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	83
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	62
4	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	58
5	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

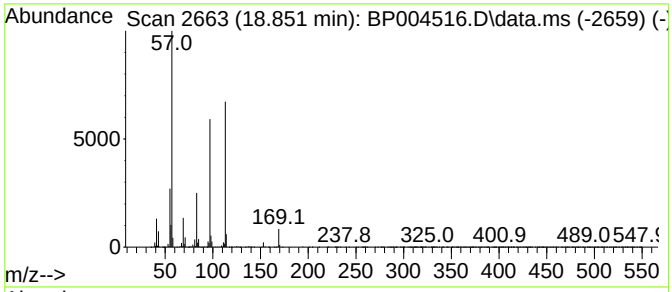
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

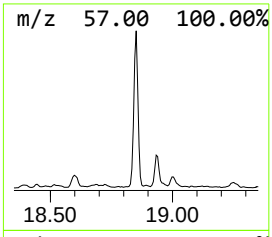
****

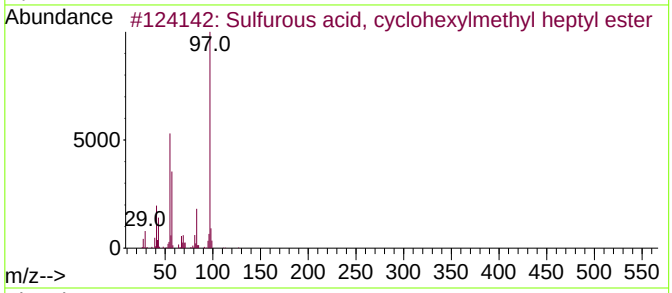
Peak Number 5 unknown18.851 Concentration Rank 3

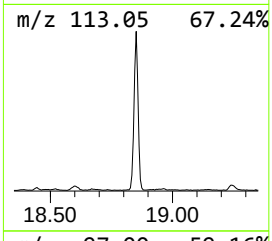
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	4.16 ng	619372	Phenanthrene-d10	17.222

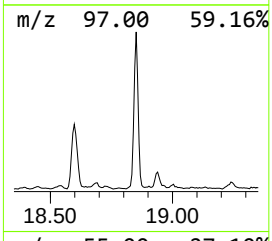
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	47
2	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	38
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	38
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35

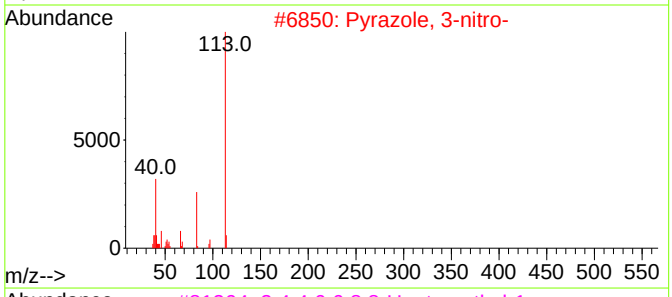


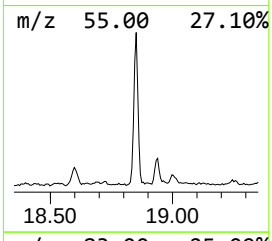


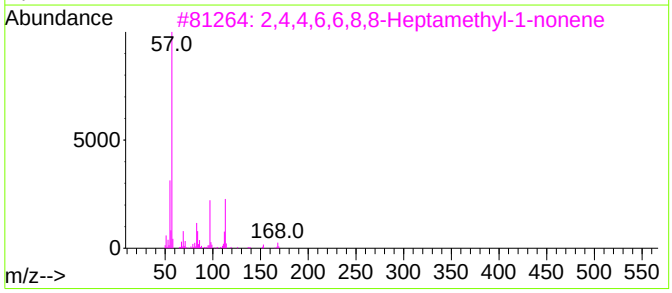


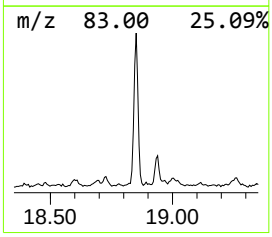












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

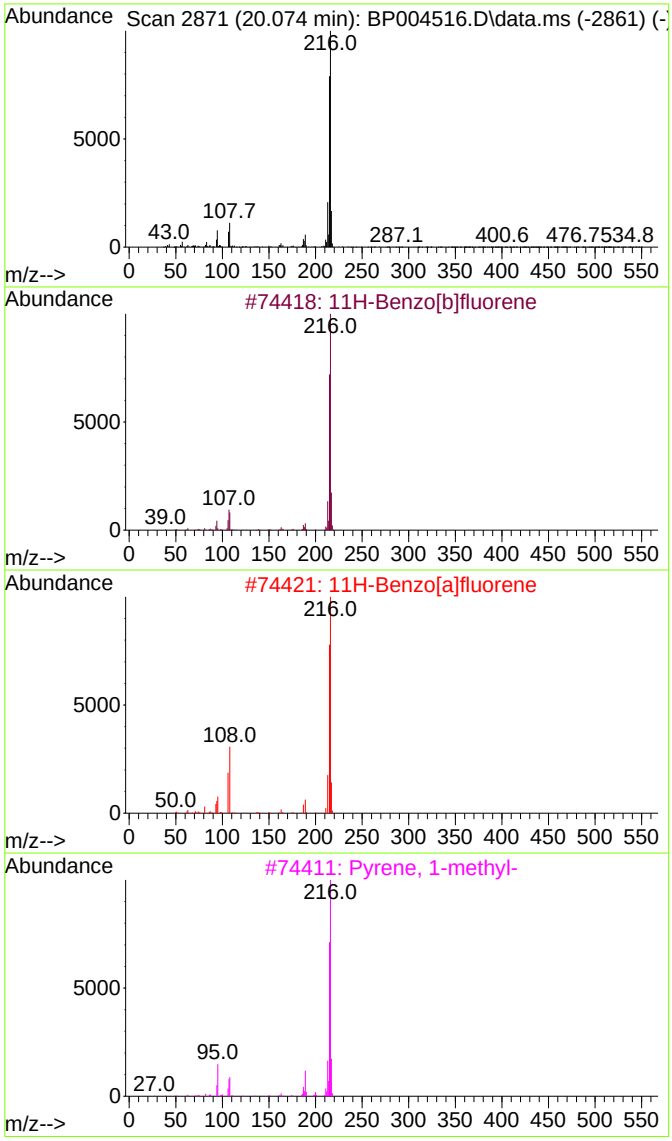
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

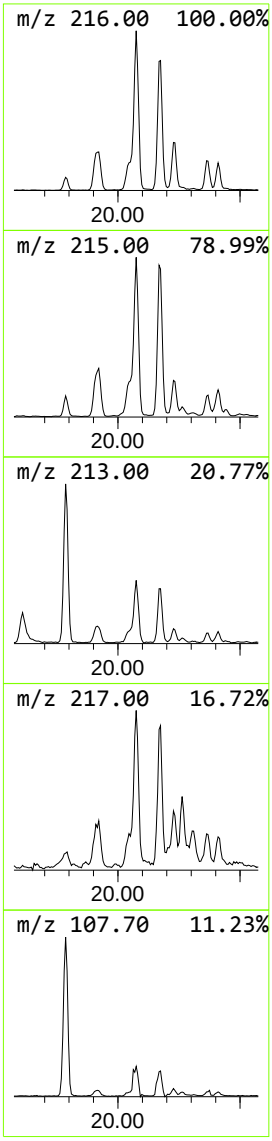
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.075	2.29 ng	512532	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91





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Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

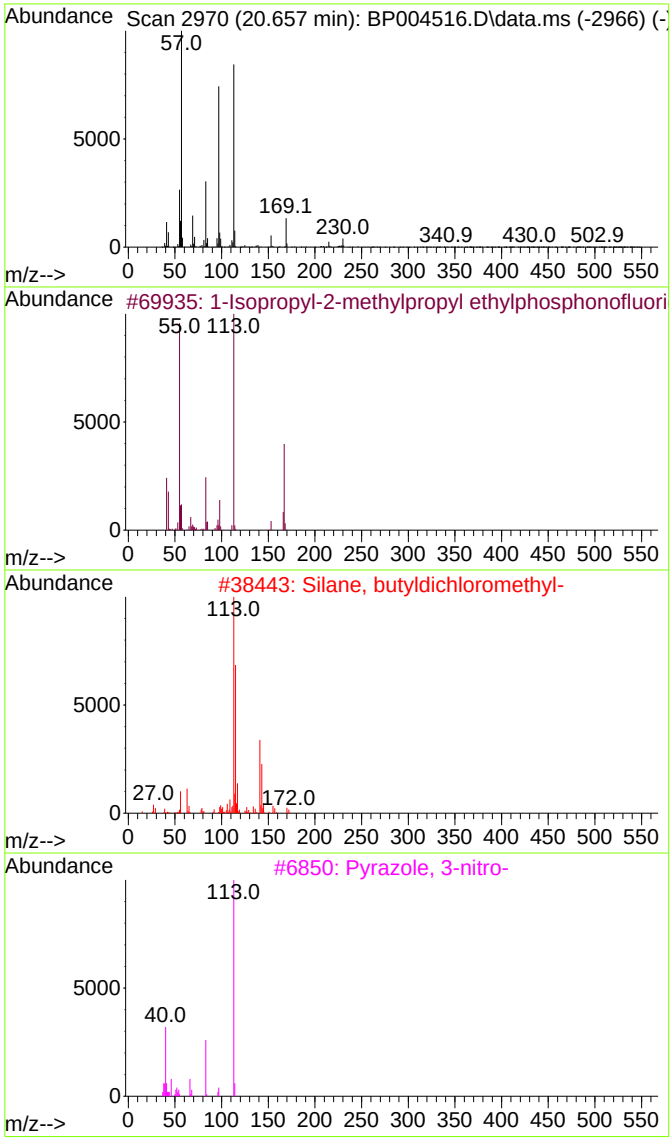
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

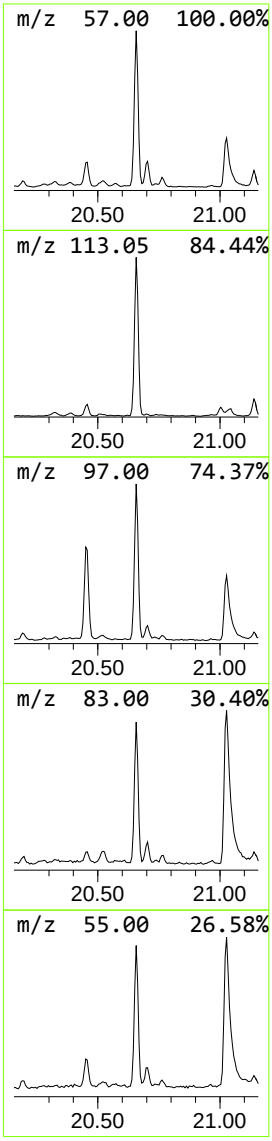
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown20.657 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.657	3.15 ng	705121	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropyl-2-methylpropyl ethyl...	210	C9H20FO2P	1000298-33-2	32
2	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	27
3	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	25
5	2-Iodo-6-methylheptane	240	C8H17I	088373-60-8	25





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Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

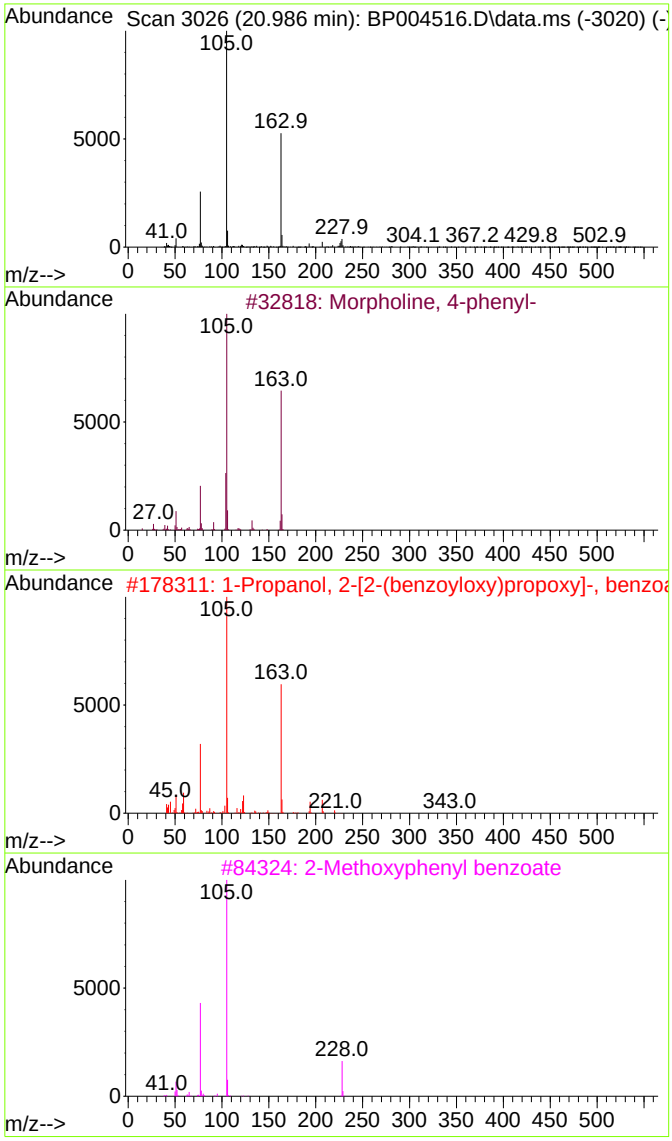
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

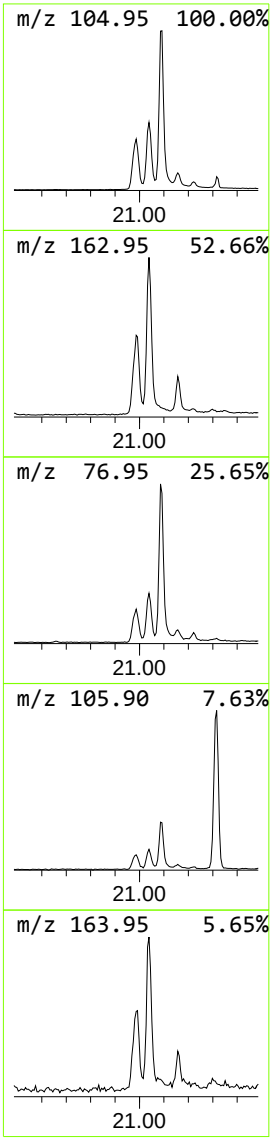
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Morpholine, 4-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	2.05 ng	459349	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40
3	2-Methoxyphenyl benzoate	228	C14H12O3	000531-37-3	35
4	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	33
5	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	28





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Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

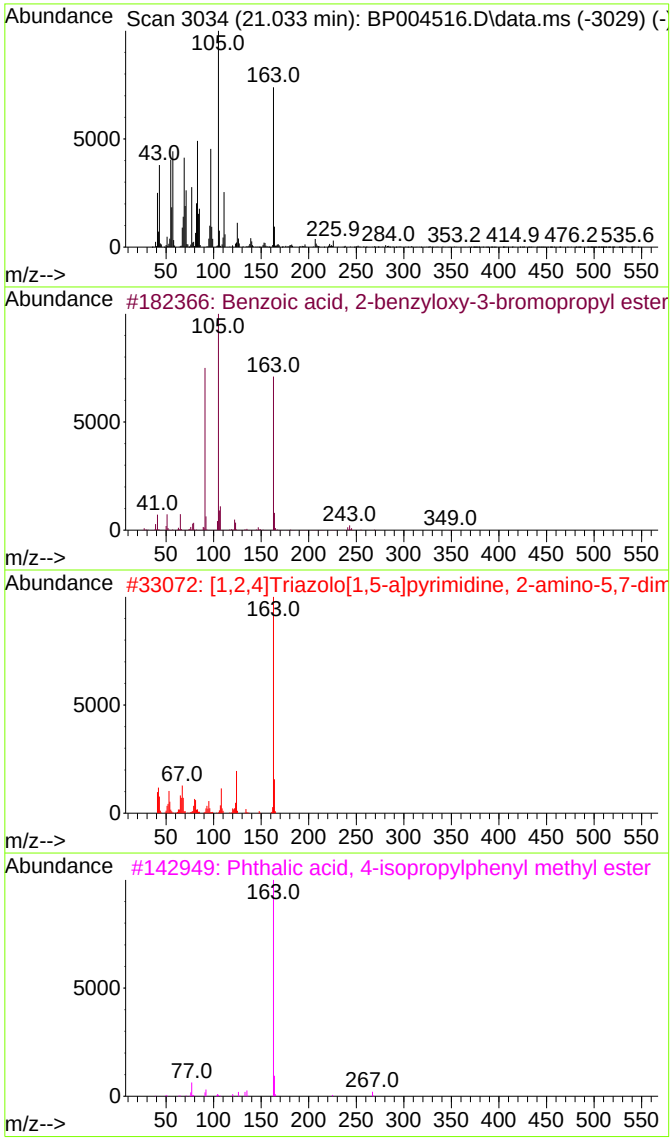
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

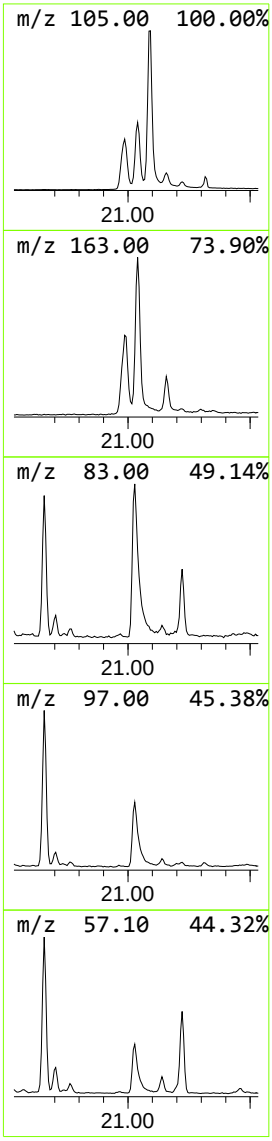
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 unknown21.033 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	6.05 ng	1354360	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	27
2	[1,2,4]Triazolo[1,5-a]pyrimidine...	163	C7H9N5	007135-02-6	22
3	Phthalic acid, 4-isopropylphenyl...	298	C18H18O4	1000315-65-7	22
4	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	16
5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	16





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Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

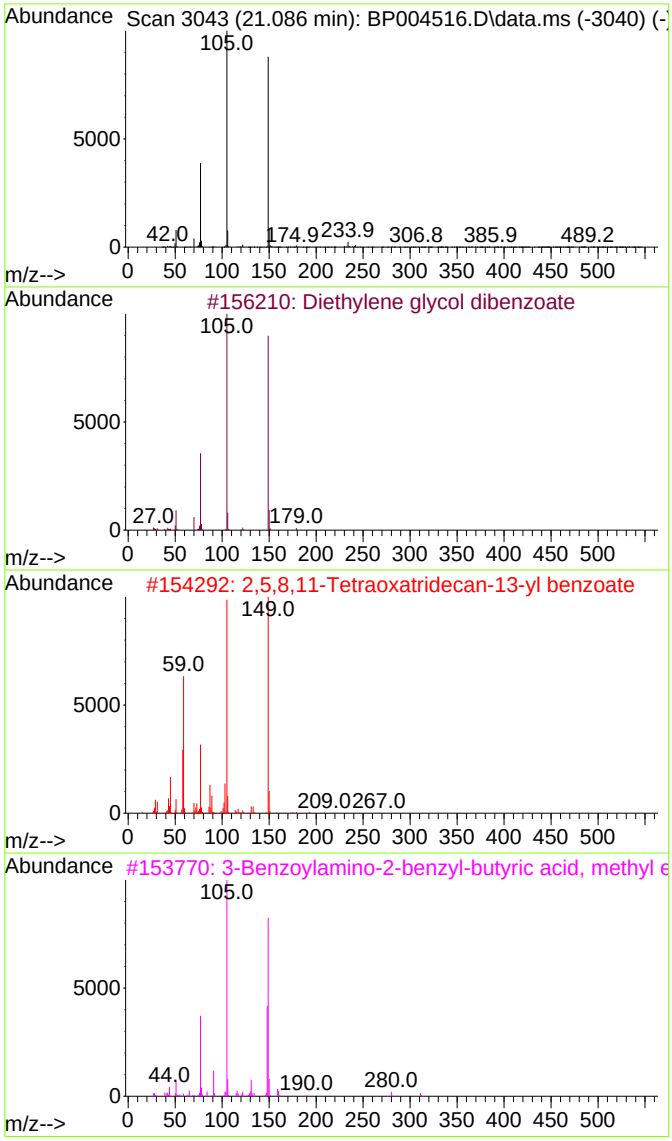
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

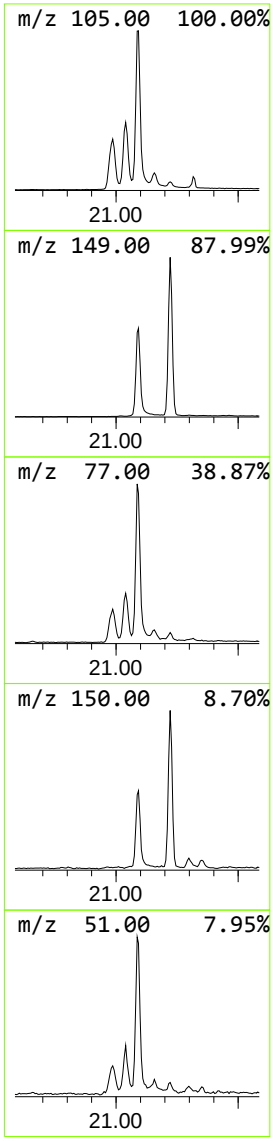
****

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	3.88 ng	868162	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
3	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011221\
Data File : BP004516.D
Acq On : 12 Jan 2021 21:37
Operator : CG/JU
Sample : M1075-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11977

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.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...	18.092	2.6	ng	383973	4	17.222	2980580	20.0
Anthracene, 2-m...	18.139	2.2	ng	331168	4	17.222	2980580	20.0
4H-Cyclopenta[d...	18.286	5.1	ng	759555	4	17.222	2980580	20.0
5,16[1',2']:8,1...	18.580	2.2	ng	325131	4	17.222	2980580	20.0
unknown18.851	18.851	4.2	ng	619372	4	17.222	2980580	20.0
11H-Benzo[b]flu...	20.075	2.3	ng	512532	5	21.316	4477650	20.0
unknown20.657	20.657	3.1	ng	705121	5	21.316	4477650	20.0
Morpholine, 4-p...	20.986	2.0	ng	459349	5	21.316	4477650	20.0
unknown21.033	21.033	6.0	ng	1354360	5	21.316	4477650	20.0
Diethylene glyc...	21.086	3.9	ng	868162	5	21.316	4477650	20.0