LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-01-COMP

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: BP005561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.799	284	291	298	rBV2	24138	38409	2.74%	0.534%
2	5.270	364	371	386	rBV	145863	246897	17.63%	3.430%
3	6.875	638	644	659	rBV	203119	363440	25.96%	5.050%
4	7.675	771	780	789	rBV	76195	129739	9.27%	1.803%
5	8.846	971	979	993	rBV	148061	260250	18.59%	3.616%
6	10.469	1243	1255	1261	rBV	82240	150521	10.75%	2.091%
7	12.946	1670	1676	1695	rVB	471292	669255	47.80%	9.299%
8	13.646	1791	1795	1801	rBV6	8320	16403	1.17%	0.228%
9	13.799	1815	1821	1826	rBV	48993	74248	5.30%	1.032%
10	14.051	1856	1864	1872	rBV2	8675	21755	1.55%	0.302%
11	14.328	1904	1911	1917	rVV	142215	201732	14.41%	2.803%
12	14.387	1917	1921	1930	rVB2	18314	28817	2.06%	0.400%
13	14.728	1969	1979	1985	rBV	17571	33202	2.37%	0.461%
14	15.381	2085	2090	2095	rBV	25566	37074	2.65%	0.515%
15	15.681	2136	2141	2147	rVB5	8924	16483	1.18%	0.229%
16	15.828	2160	2166	2173	rBV	214896	329013	23.50%	4.571%
17	16.069	2200	2207	2212	rVB4	19790	39751	2.84%	0.552%
18	16.898	2343	2348	2356	rVB3	20714	39471	2.82%	0.548%
19	17.087	2374	2380	2383	rBV	207092	271031	19.36%	3.766%
20	17.128	2383	2387	2393	rVB	156637	213561	15.25%	2.967%
21	17.222	2398	2403	2408	rVB	52086	74937	5.35%	1.041%
22	17.504	2447	2451	2457	rBV2	13843	29261	2.09%	0.407%
23	17.587	2462	2465	2471	rVB6	9495	14344	1.02%	0.199%
24	17.957	2525	2528	2530	rBV	24408	26044	1.86%	0.362%
25	18.004	2530	2536	2542	rVB3	37704	80828	5.77%	1.123%
26	18.087	2547	2550	2553	rVV2	15992	19769	1.41%	0.275%
27	18.145	2556	2560	2564	rVV3	45760	74599	5.33%	1.036%
28	18.187	2564	2567	2570	rVB	21090	25192	1.80%	0.350%
29	18.263	2577	2580	2583	rBV4	17929	20275	1.45%	0.282%
30	18.445	2607	2611	2616	rBV	25697	42151	3.01%	0.586%
31	18.651	2644	2646	2649	rBV4	11360	14195	1.01%	0.197%
32	18.845	2676	2679	2682	rBV2	26815	34832	2.49%	0.484%
33	19.104	2719	2723	2730	rBV	323738	417977	29.85%	5.807%
34	19.457	2775	2783	2793	rBV	274292	500194	35.73%	6.950%
35	19.534	2793	2796	2801	rVV3	27843	41456	2.96%	0.576%
36	19.657	2812	2817	2822	rVB	1228786	1400100	100.00%	19.453%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-01-COMP

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	20.039	2880	2882	2886	rVB	47218	50402	3.60%	0.700%
38	20.439	2948	2950	2955	rVB6	43386	43853	3.13%	0.609%
39	20.898	3025	3028	3036	rVB5	103516	180527	12.89%	2.508%
40	21.186	3071	3077	3081	rBV2	386374	715633	51.11%	9.943%
41	21.222	3081	3083	3090	rVB	184103	209651	14.97%	2.913%

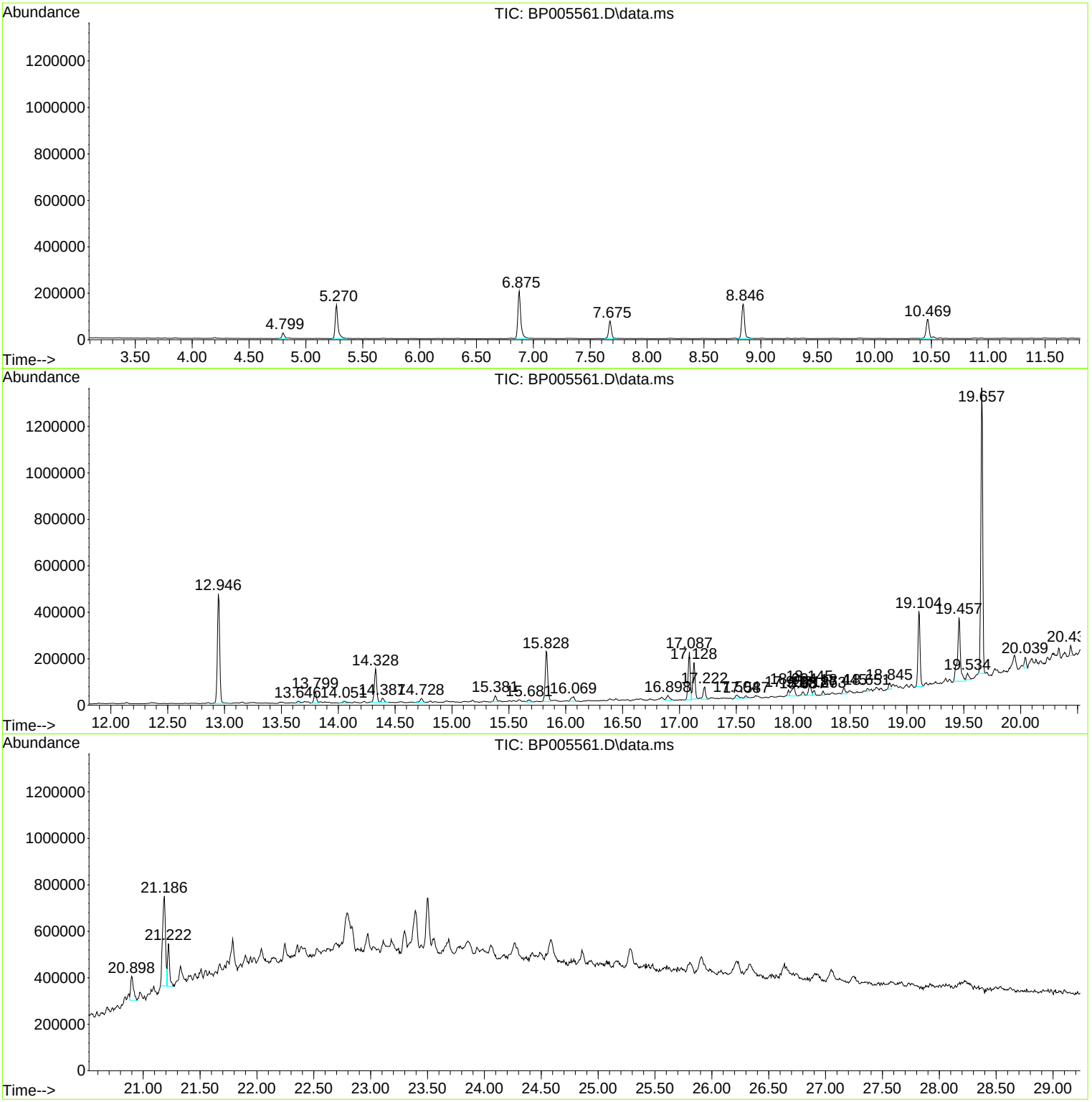
Sum of corrected areas: 7197272

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

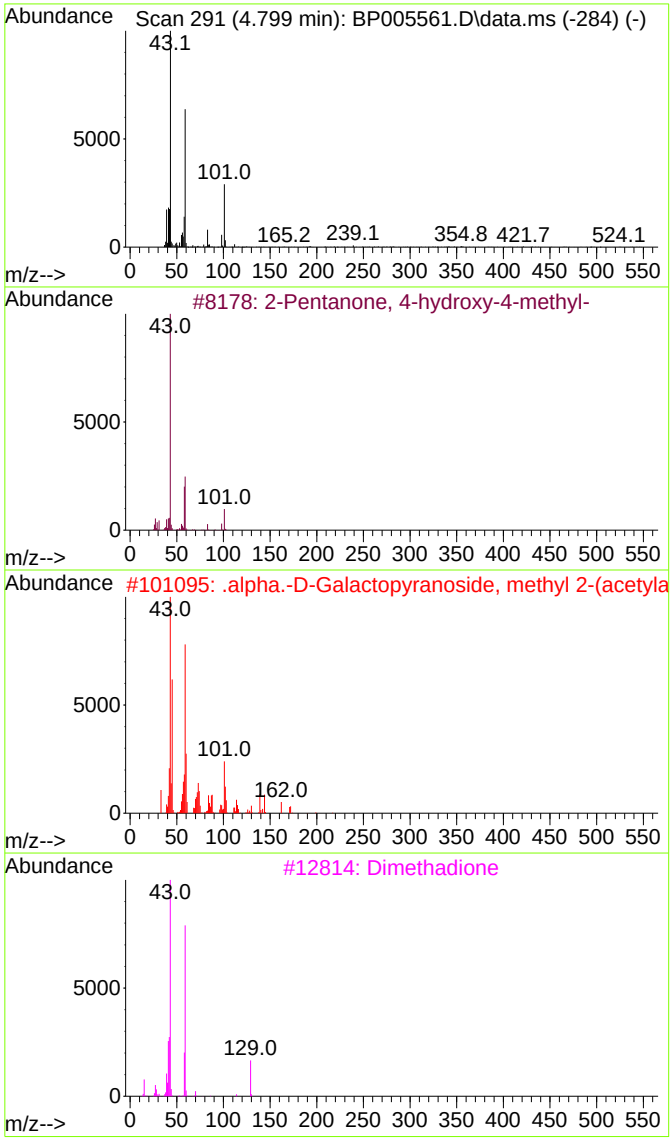
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

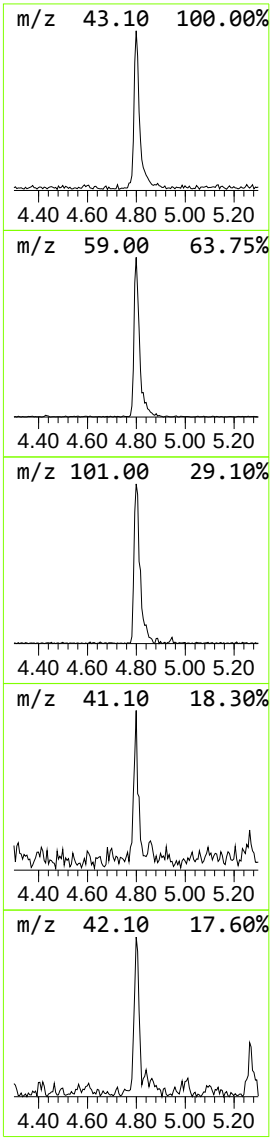
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.799	5.92 ng	38409	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	Dimethadione	129	C5H7NO3	000695-53-4	38
4	Guanidine	59	CH5N3	000113-00-8	37
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-01-COMP

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

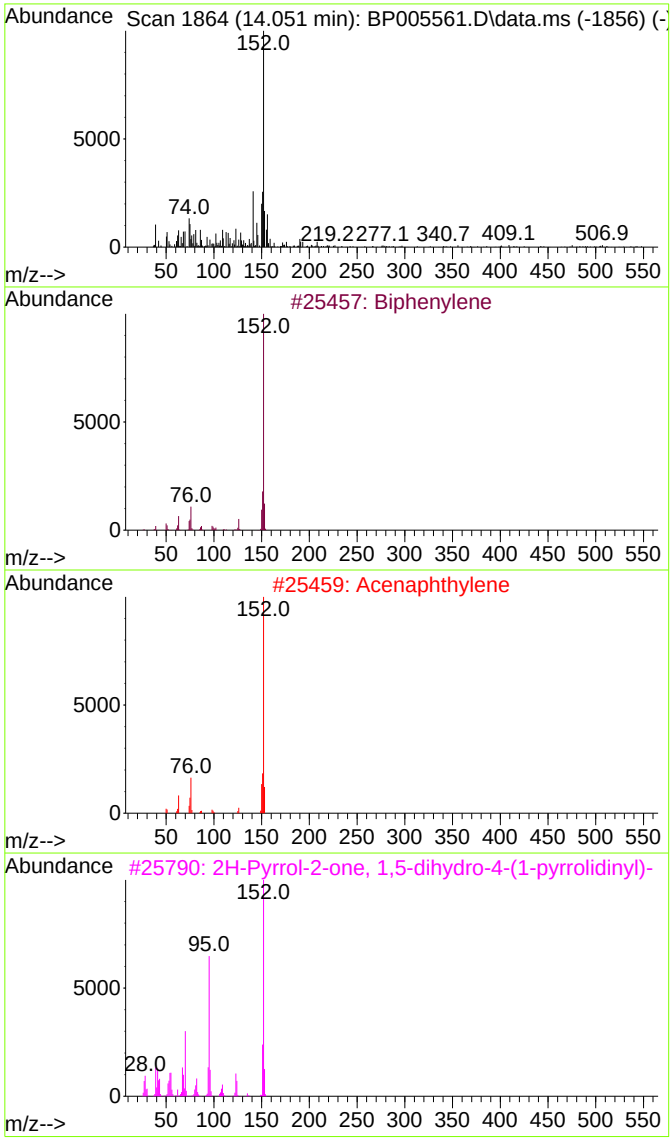
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

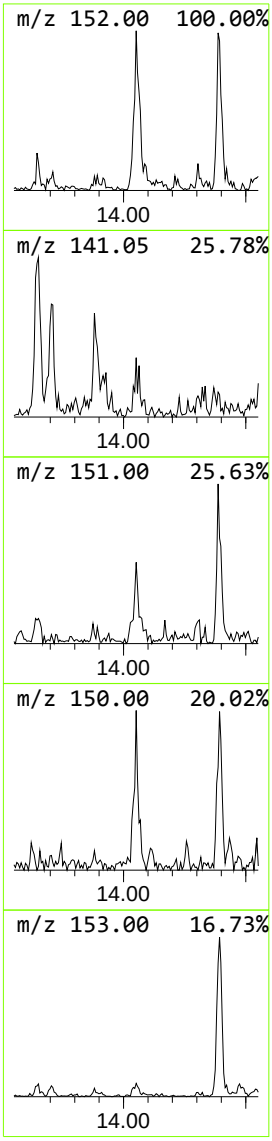
****

Peak Number 2 Biphenylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.051	2.16 ng	21755	Acenaphthene-d10	14.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenylene	152	C12H8	000259-79-0	50
2	Acenaphthylene	152	C12H8	000208-96-8	49
3	2H-Pyrrol-2-one, 1,5-dihydro-4-(...	152	C8H12N2O	105776-93-0	49
4	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	47
5	5-Chlorobenzimidazole	152	C7H5ClN2	004887-82-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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

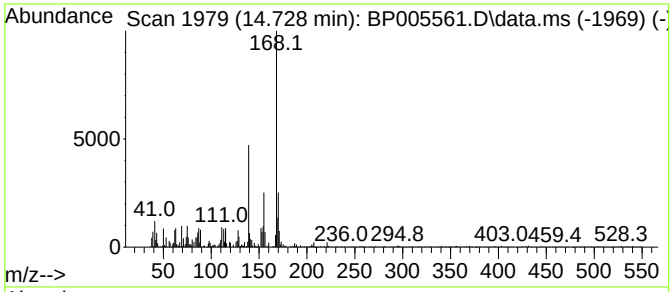
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

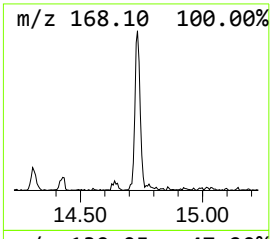
****

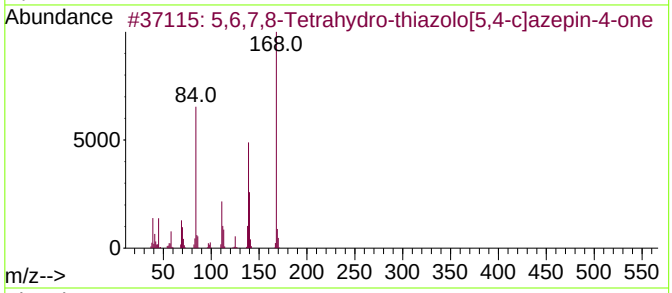
Peak Number 3 5,6,7,8-Tetrahydro-thiazolo... Concentration Rank 5

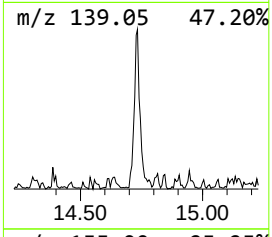
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.728	3.29 ng	33202	Acenaphthene-d10	14.328

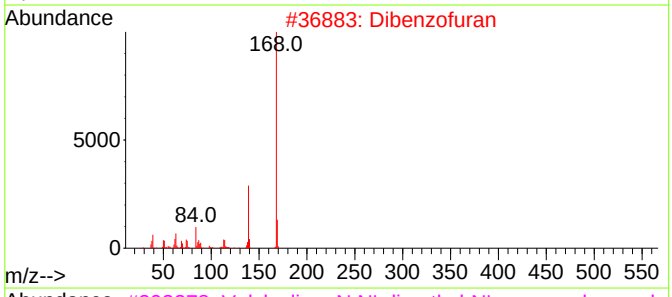
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6,7,8-Tetrahydro-thiazolo[5,4-...	168	C7H8N2OS	1000317-75-4	58
2	Dibenzofuran	168	C12H8O	000132-64-9	50
3	Valylvaline, N,N'-dimethyl-N'-pr...	382	C20H34N2O5	1000328-74-2	38
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	38
5	1-Naphthalen-1-yl-ethylideneamine	169	C12H11N	1000187-76-0	38

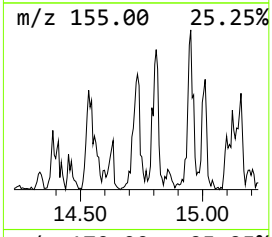


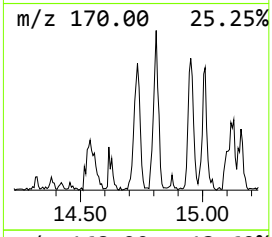


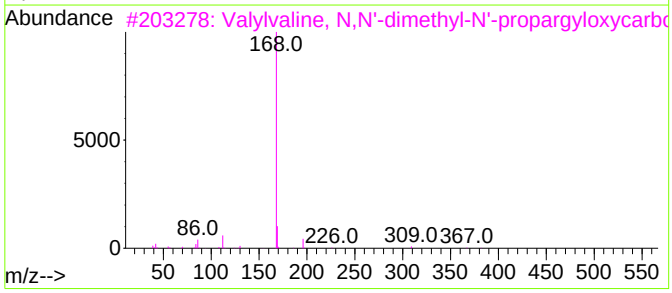


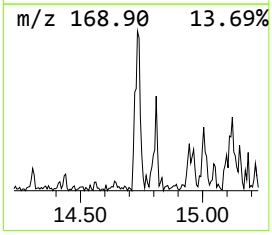












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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

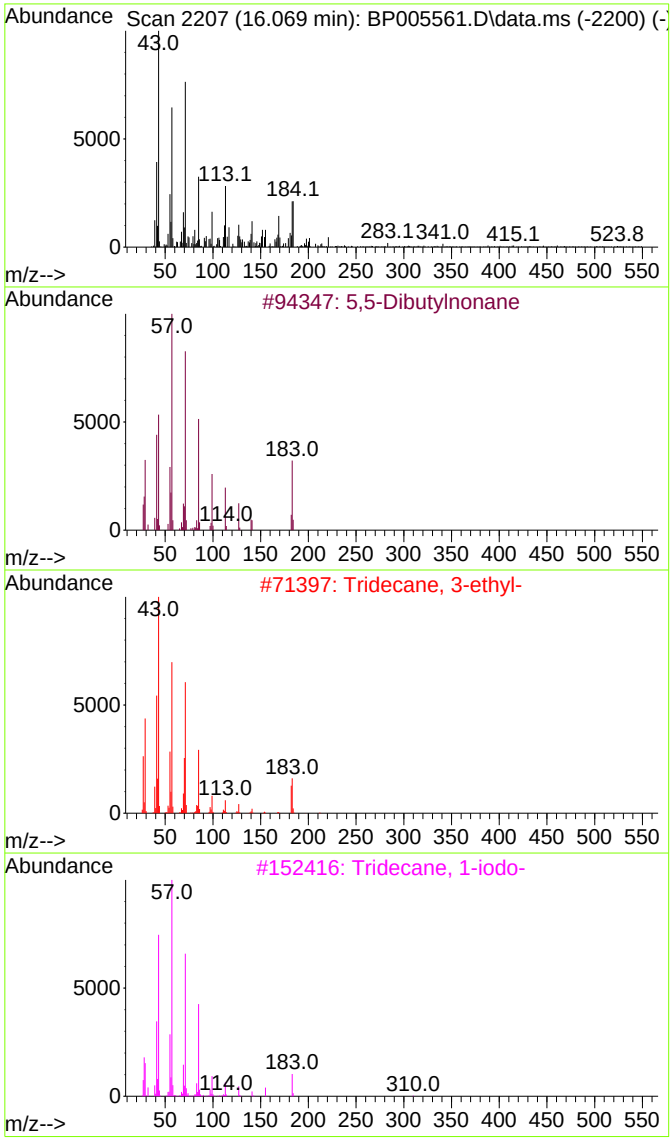
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

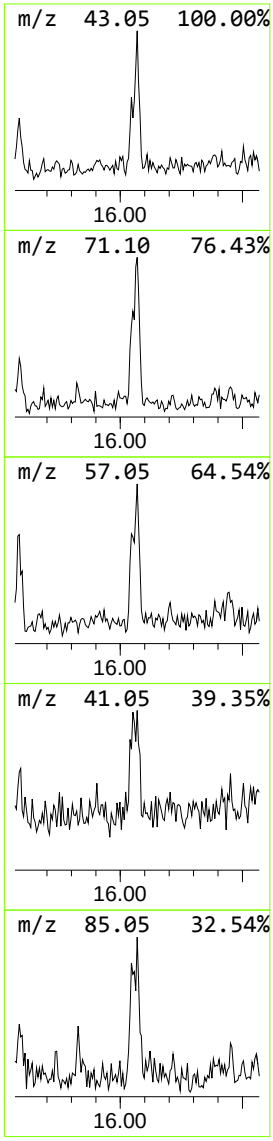
****

Peak Number 4 5,5-Dibutylnonane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.069	2.93 ng	39751	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dibutylnonane	240	C17H36	006008-17-9	64
2	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	58
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	55
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	49
5	l-Threitol, 2-O-nonyl-	248	C13H28O4	163776-15-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

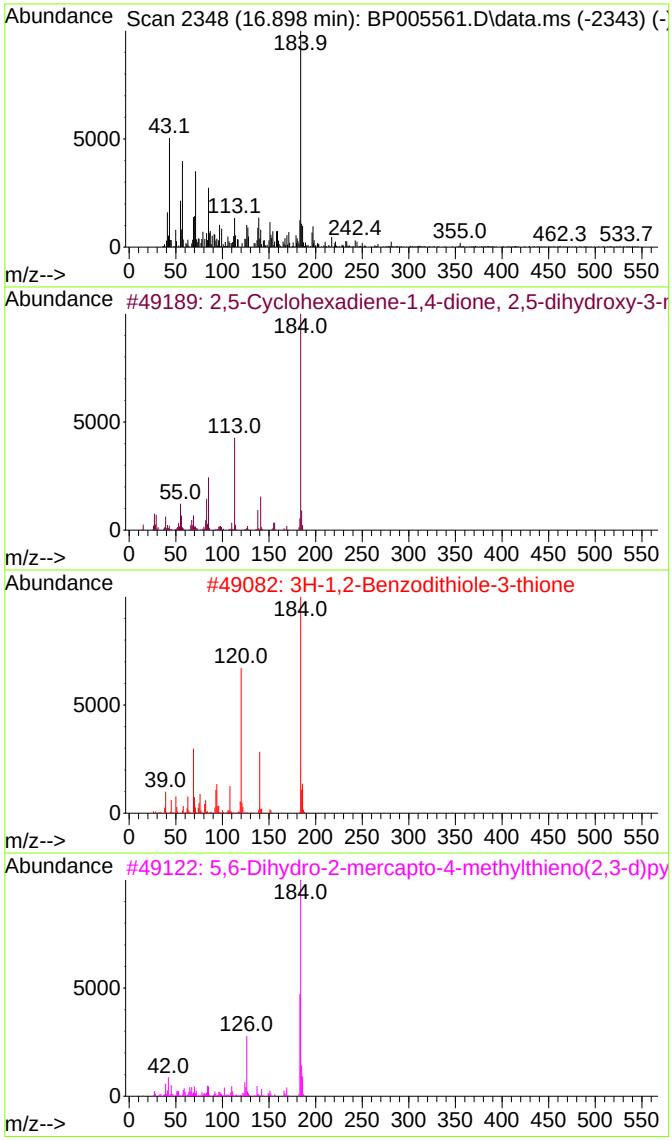
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

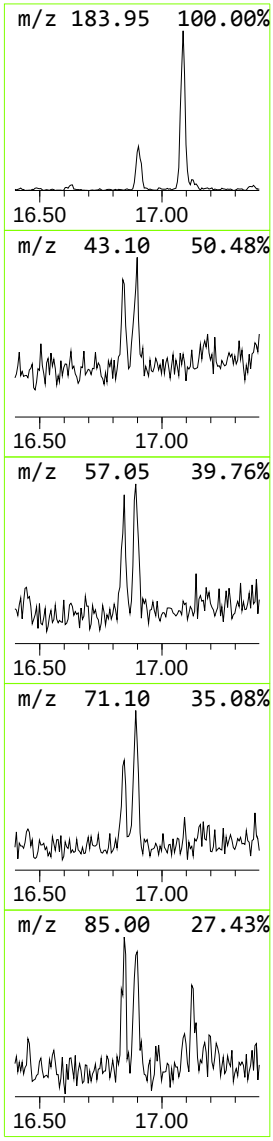
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	2.91 ng	39471	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	184	C8H8O5	000085-23-4	64
2	3H-1,2-Benzodithiole-3-thione	184	C7H4S3	003354-42-5	58
3	5,6-Dihydro-2-mercapto-4-methylt...	184	C7H8N2S2	005909-38-6	58
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	53
5	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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

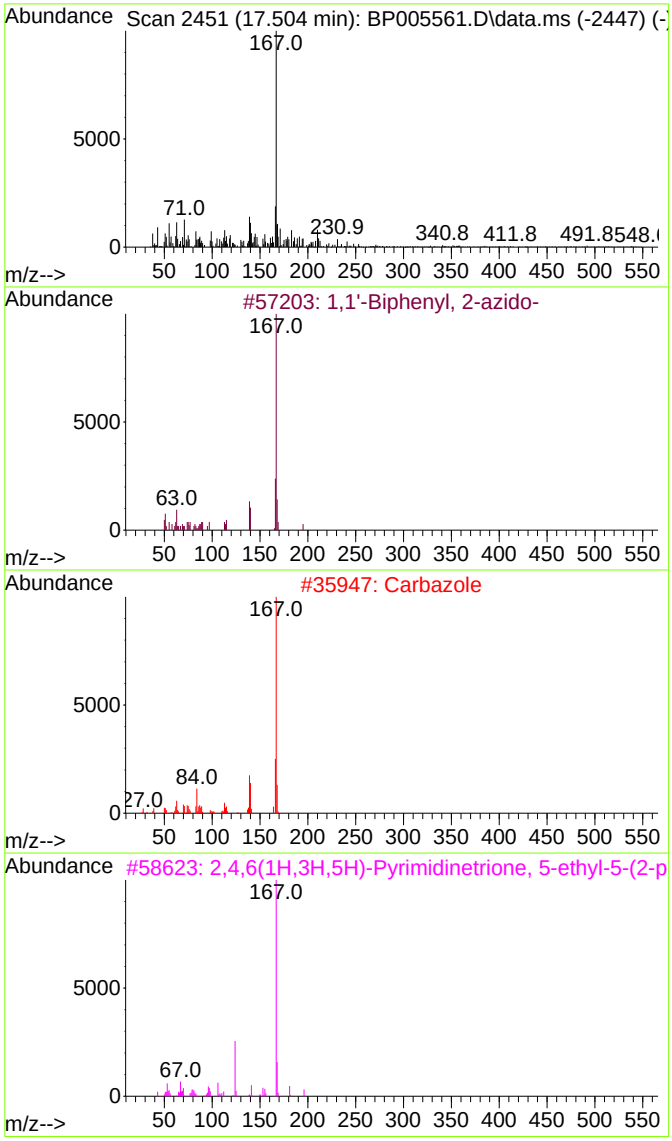
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

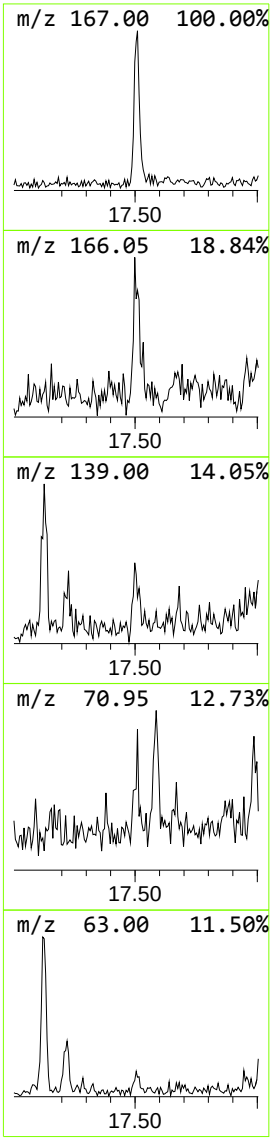
****

Peak Number 6 1,1'-Biphenyl, 2-azido- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.504	2.16 ng	29261	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	76
2	Carbazole	167	C12H9N	000086-74-8	68
3	2,4,6(1H,3H,5H)-Pyrimidinetrione...	196	C9H12N2O3	002373-84-4	64
4	.beta.-d-Mannofuranoside, 2,3:5,...	422	C23H28B2O6	1000154-76-6	64
5	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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

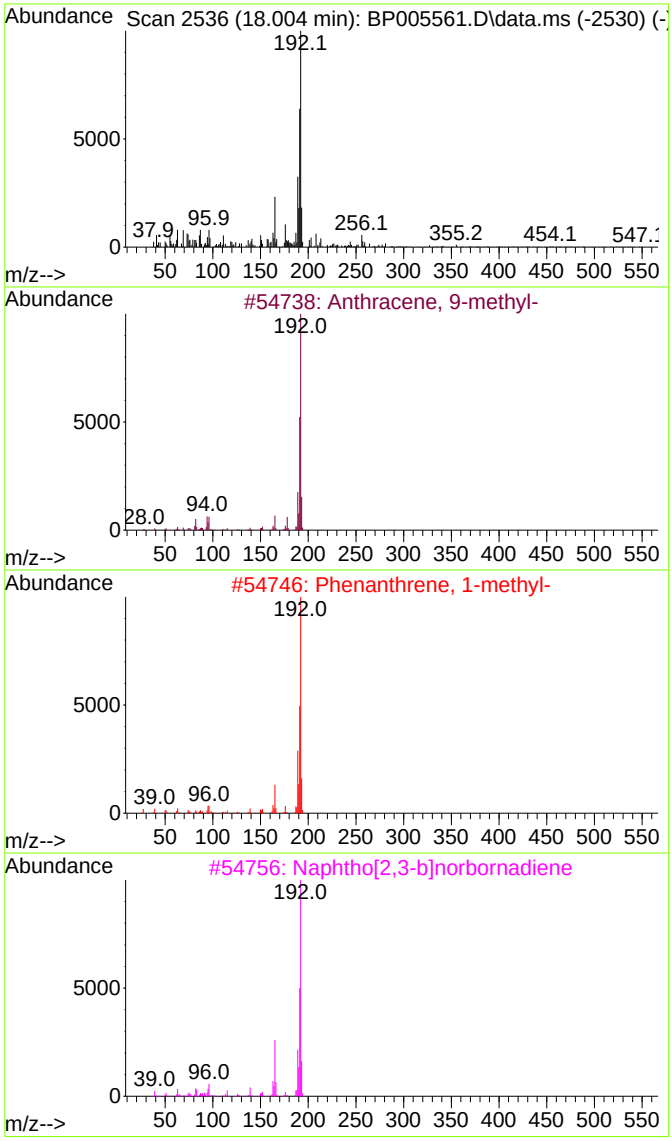
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

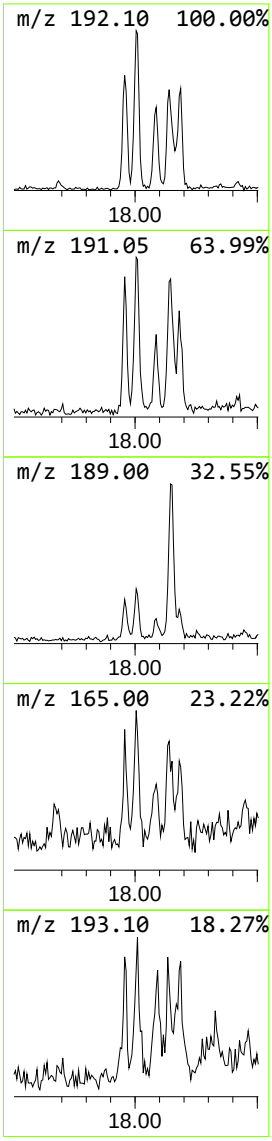
****

Peak Number 7 Anthracene, 9-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	5.96 ng	80828	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	81
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	81





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Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

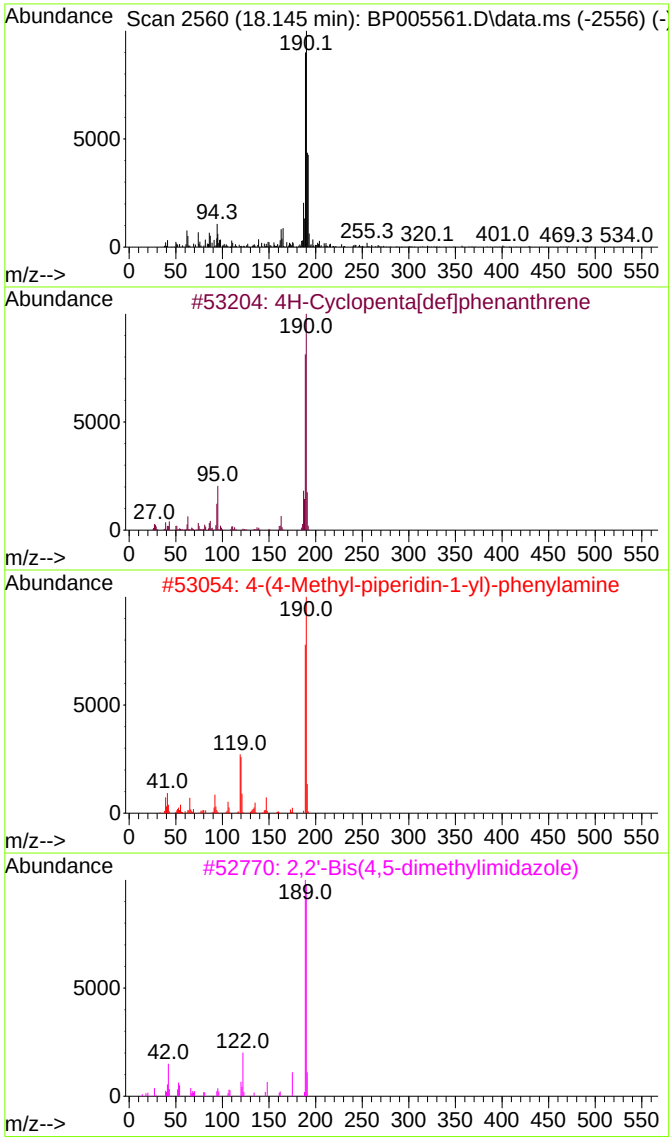
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

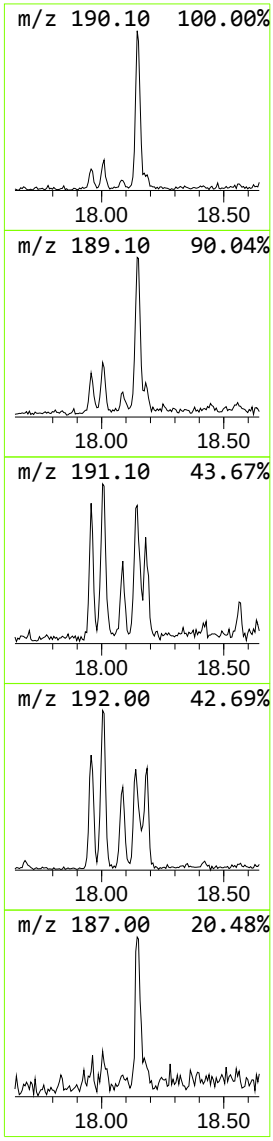
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	5.50 ng	74599	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	47
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	25
5	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	25





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Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

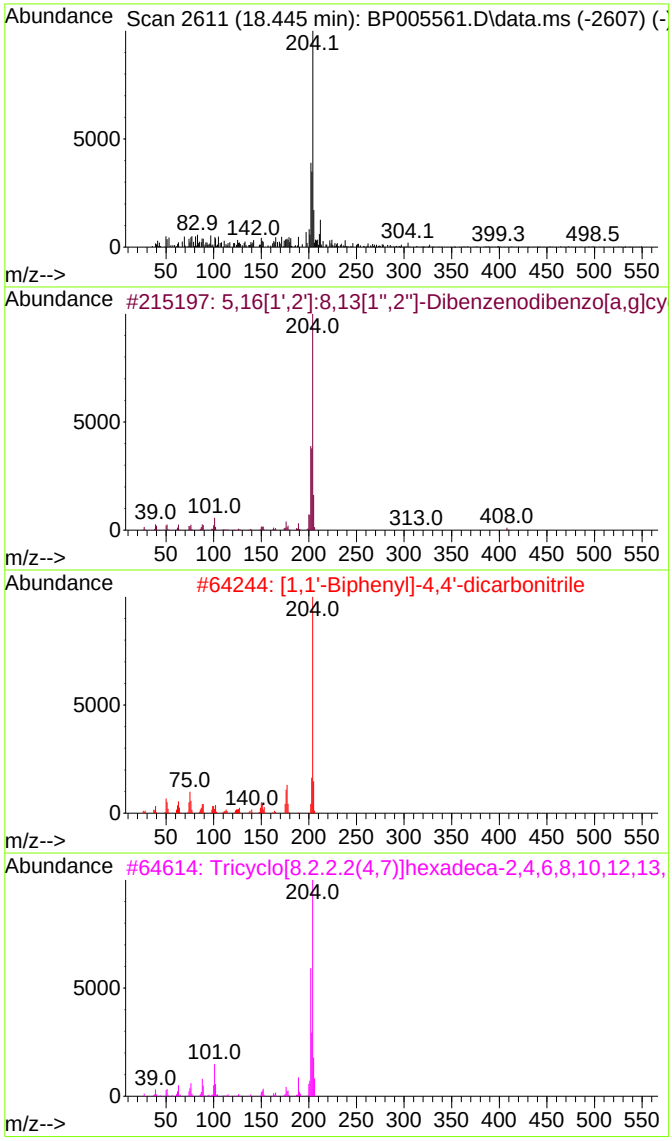
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

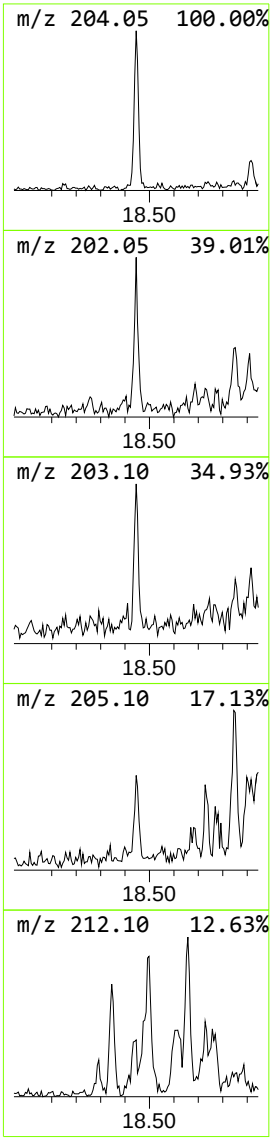
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.445	3.11 ng	42151	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	80
2	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	53
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	53
4	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	53
5	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	50





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Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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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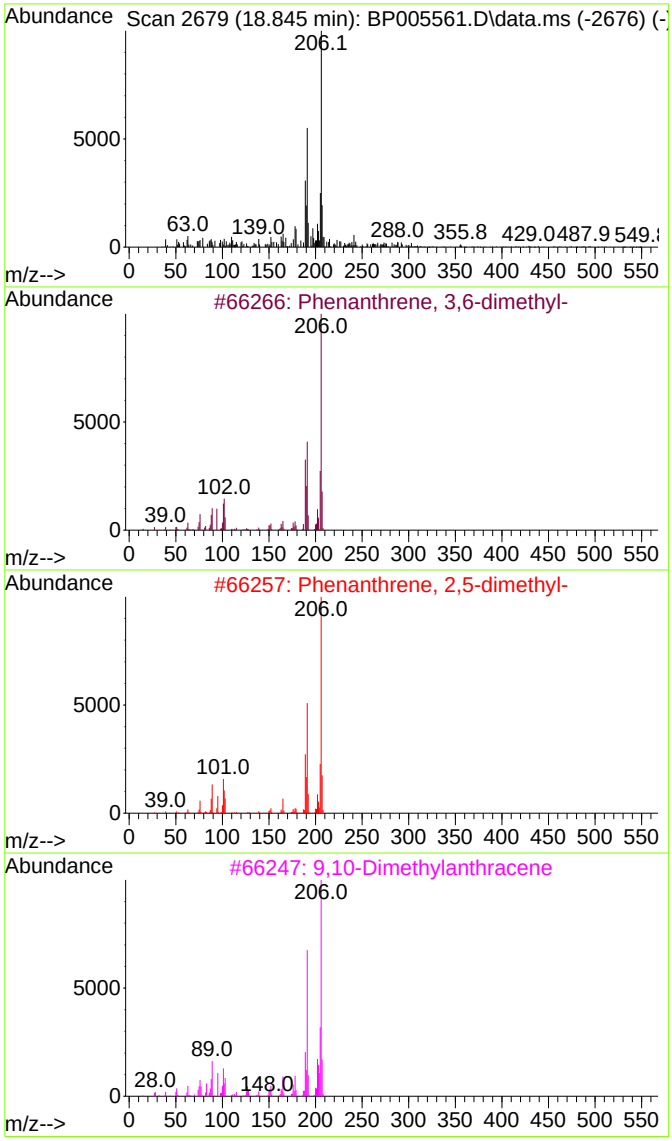
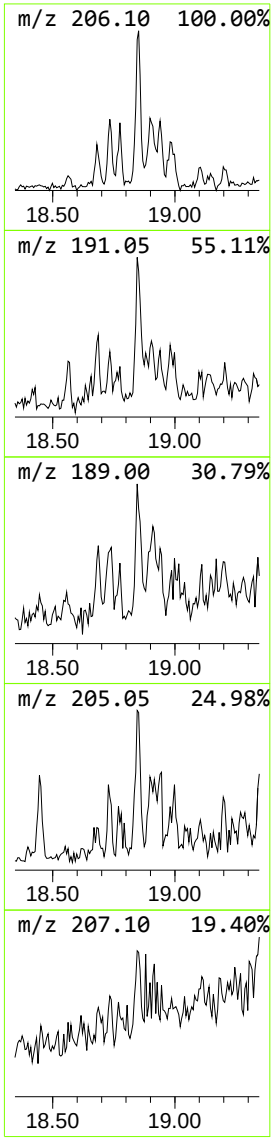
Peak Number 10 Phenanthrene, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.845	2.57 ng	34832	Phenanthrene-d10	17.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	94
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	81
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	78
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	72





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Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-01-COMP

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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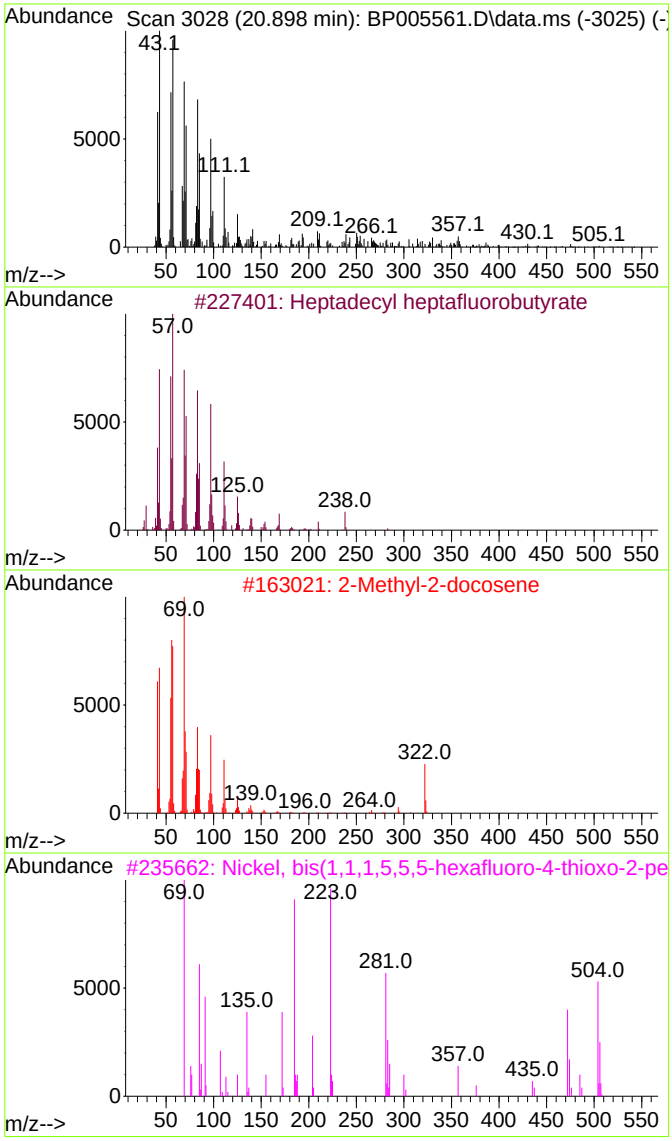
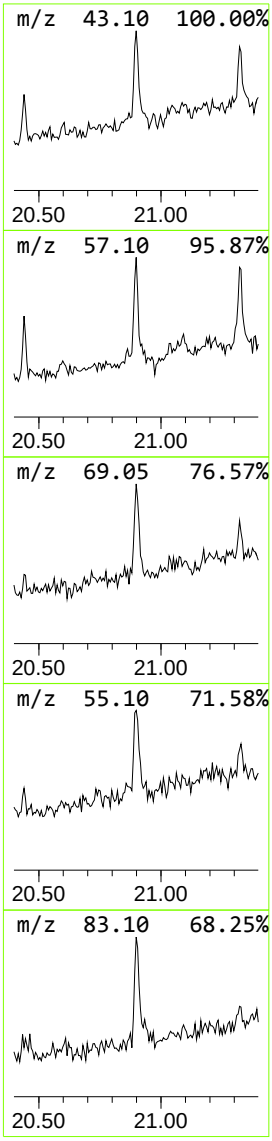
Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.898	5.05 ng	180527	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2	2-Methyl-2-docosene	322	C23H46	1000131-16-9	86
3	Nickel, bis(1,1,1,5,5,5-hexafluo...	504	C10H2F12NiO2S2	031541-97-6	83
4	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	81
5	1-Triacontanol	438	C30H62O	000593-50-0	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005561.D
Acq On : 14 May 2021 22:05
Operator : CG/JU
Sample : M2392-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-01-COMP

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
2-Pentanone, 4-...	4.799	5.9	ng	38409	1	7.675	129739	20.0
Biphenylene	14.051	2.2	ng	21755	3	14.328	201732	20.0
5,6,7,8-Tetrahy...	14.728	3.3	ng	33202	3	14.328	201732	20.0
5,5-Dibutylnonane	16.069	2.9	ng	39751	4	17.087	271031	20.0
2,5-Cyclohexadi...	16.898	2.9	ng	39471	4	17.087	271031	20.0
1,1'-Biphenyl, ...	17.504	2.2	ng	29261	4	17.087	271031	20.0
Anthracene, 9-m...	18.004	6.0	ng	80828	4	17.087	271031	20.0
4H-Cyclopenta[d...	18.145	5.5	ng	74599	4	17.087	271031	20.0
5,16[1',2']:8,1...	18.445	3.1	ng	42151	4	17.087	271031	20.0
Phenanthrene, 3...	18.845	2.6	ng	34832	4	17.087	271031	20.0
Heptadecyl hept...	20.898	5.0	ng	180527	5	21.186	715633	20.0