LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

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_F\Methods\8270-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.493	573	578	595	rBV	1037450	1448501	79.95%	8.523%
2	6.504	745	750	769	rBV	1142442	1538909	84.94%	9.055%
3	6.869	807	812	819	rBV	331540	399503	22.05%	2.351%
4	7.434	902	908	917	rBV	723555	978258	53.99%	5.756%
5	7.686	943	951	963	rBV	14460	28744	1.59%	0.169%
6	8.151	1021	1030	1044	rBV	385022	540358	29.82%	3.179%
7	8.863	1147	1151	1158	rVB	13477	18984	1.05%	0.112%
8	8.963	1163	1168	1175	rVV	19309	25858	1.43%	0.152%
9	9.222	1207	1212	1222	rBV	1432775	1811813	100.00%	10.660%
10	9.492	1253	1258	1264	rBV	16159	27933	1.54%	0.164%
11	9.563	1266	1270	1273	rBV	24047	35344	1.95%	0.208%
12	9.680	1287	1290	1299	rVB2	11130	19441	1.07%	0.114%
13	9.904	1323	1328	1332	rBV	437033	565991	31.24%	3.330%
14	9.939	1332	1334	1342	rVB	79004	86282	4.76%	0.508%
15	10.110	1359	1363	1367	rBV	50898	66408	3.67%	0.391%
16	10.222	1378	1382	1385	rBV2	13301	19071	1.05%	0.112%
17	10.327	1392	1400	1406	rBV3	15849	34625	1.91%	0.204%
18	10.457	1417	1422	1427	rBV	61302	86090	4.75%	0.507%
19	10.522	1427	1433	1434	rVV2	11052	19153	1.06%	0.113%
20	10.539	1434	1436	1443	rVV6	16366	30278	1.67%	0.178%
21	10.616	1444	1449	1457	rVV	187936	257828	14.23%	1.517%
22	10.698	1457	1463	1477	rVV	768178	1066475	58.86%	6.275%
23	10.810	1477	1482	1489	rVB3	21966	49126	2.71%	0.289%
24	11.004	1511	1515	1518	rBV3	16123	23350	1.29%	0.137%
25	11.127	1532	1536	1538	rBV3	17154	25681	1.42%	0.151%
26	11.204	1545	1549	1552	rBV	25597	31691	1.75%	0.186%
27	11.245	1552	1556	1560	rVV2	22760	36295	2.00%	0.214%
28	11.292	1560	1564	1570	rVB	42908	64038	3.53%	0.377%
29	11.398	1576	1582	1583	rBV	420854	535284	29.54%	3.149%
30	11.422	1583	1586	1590	rVV	627570	795597	43.91%	4.681%
31	11.469	1590	1594	1600	rVB	141119	194961	10.76%	1.147%
32	11.633	1616	1622	1627	rBV2	41722	75878	4.19%	0.446%
33	11.733	1635	1639	1643	rVB3	15014	21430	1.18%	0.126%
34	11.922	1663	1671	1676	rBV2	139709	294046	16.23%	1.730%
35	11.974	1677	1680	1682	rVV	34620	43071	2.38%	0.253%
36	12.010	1682	1686	1695	rVB2	92670	181312	10.01%	1.067%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

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_F\Methods\8270-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.086	1695	1699	1704	rBV4	18690	35503	1.96%	0.209%
38	12.192	1714	1717	1720	rBV	38825	49581	2.74%	0.292%
39	12.221	1720	1722	1727	rVB	29539	37000	2.04%	0.218%
40	12.445	1757	1760	1763	rBV	45301	68320	3.77%	0.402%
41	12.539	1773	1776	1780	rBV	39639	47774	2.64%	0.281%
42	12.616	1784	1789	1793	rBV	711841	933571	51.53%	5.493%
43	12.845	1821	1828	1833	rBV	623386	940445	51.91%	5.533%
44	12.980	1845	1851	1859	rBV	1255592	1647625	90.94%	9.694%
45	14.039	2027	2031	2035	rBV2	424982	746165	41.18%	4.390%
46	15.474	2272	2275	2281	rVB	141661	221148	12.21%	1.301%
47	15.539	2283	2286	2304	rVB2	231130	479390	26.46%	2.821%
48	16.686	2477	2481	2493	rVB	152163	311806	17.21%	1.835%

Sum of corrected areas: 16995935

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
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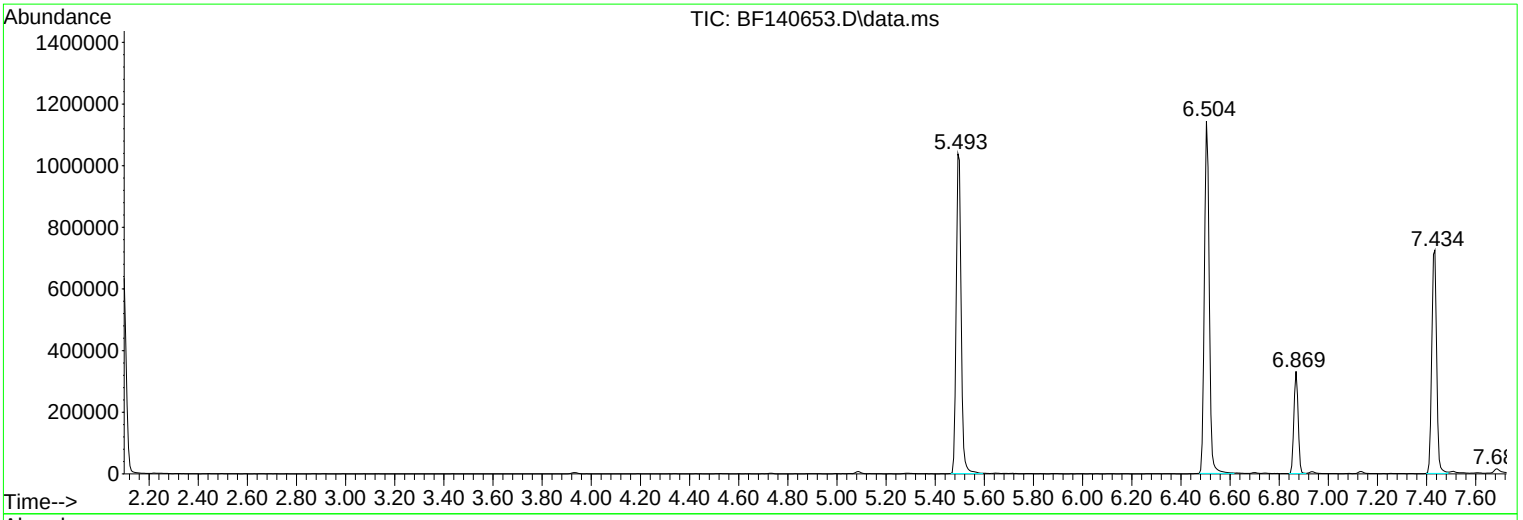
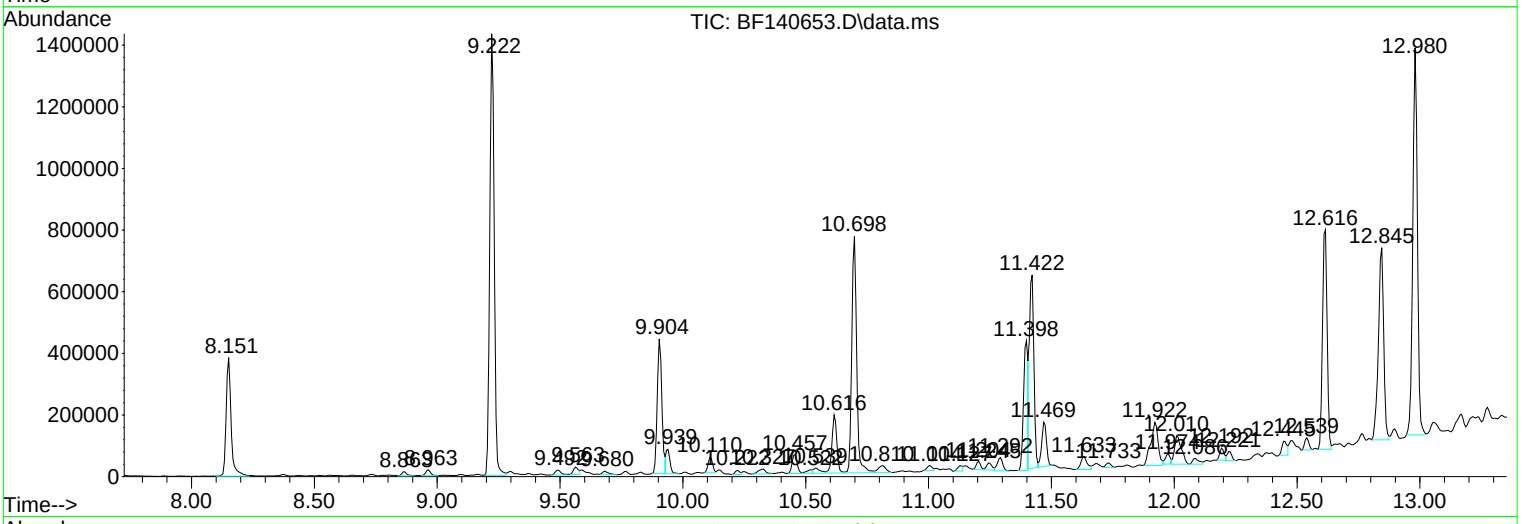
Misc :
ALS Vial : 26 Sample Multiplier: 1

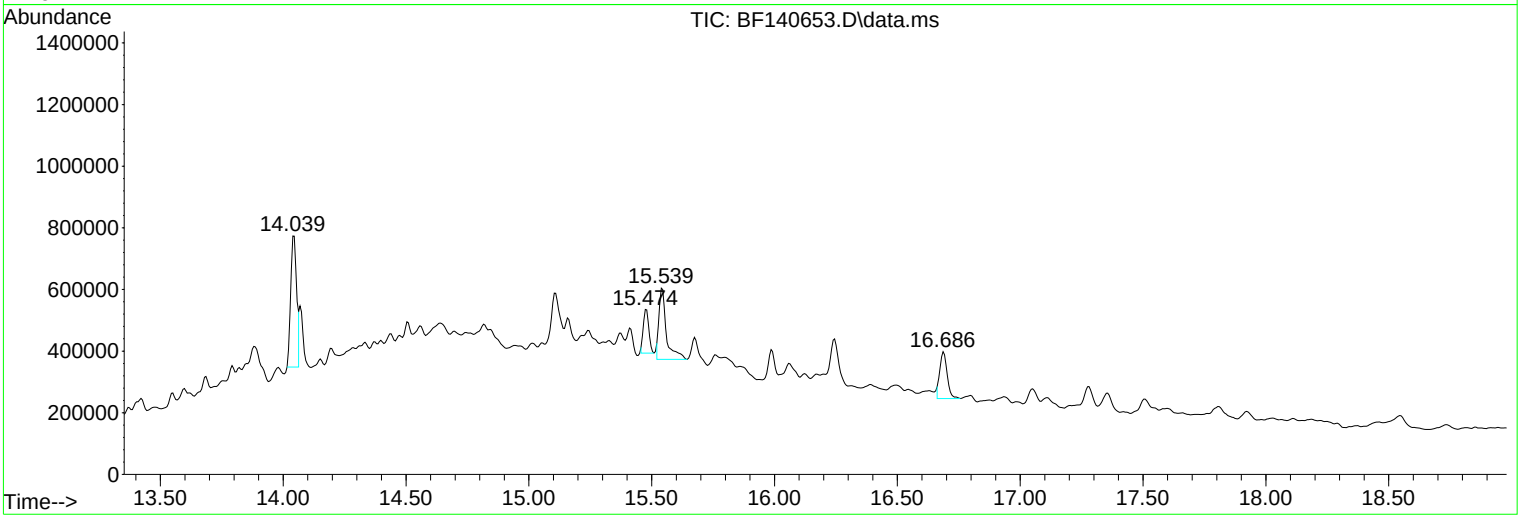
Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

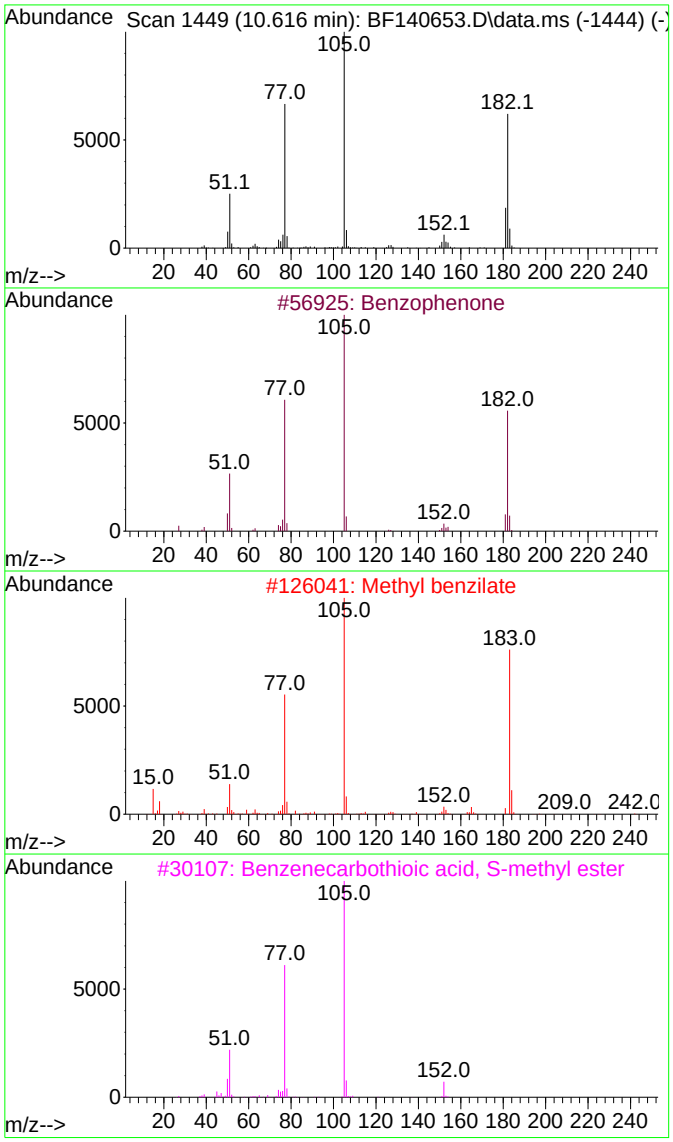
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

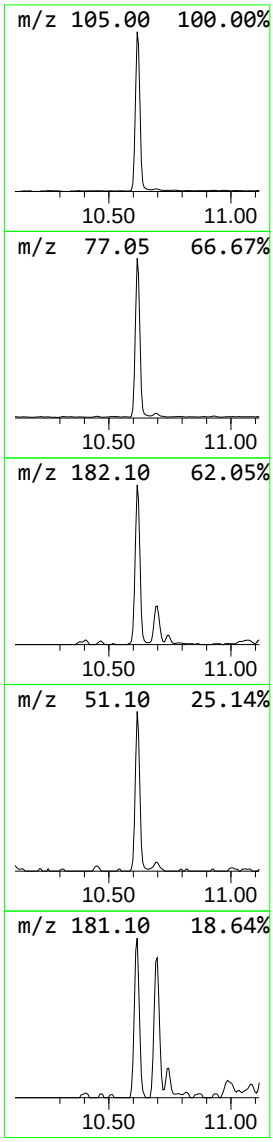
****

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	9.11 ng	257828	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Methyl benzilate	242	C15H14O3	000076-89-1	47
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	43
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

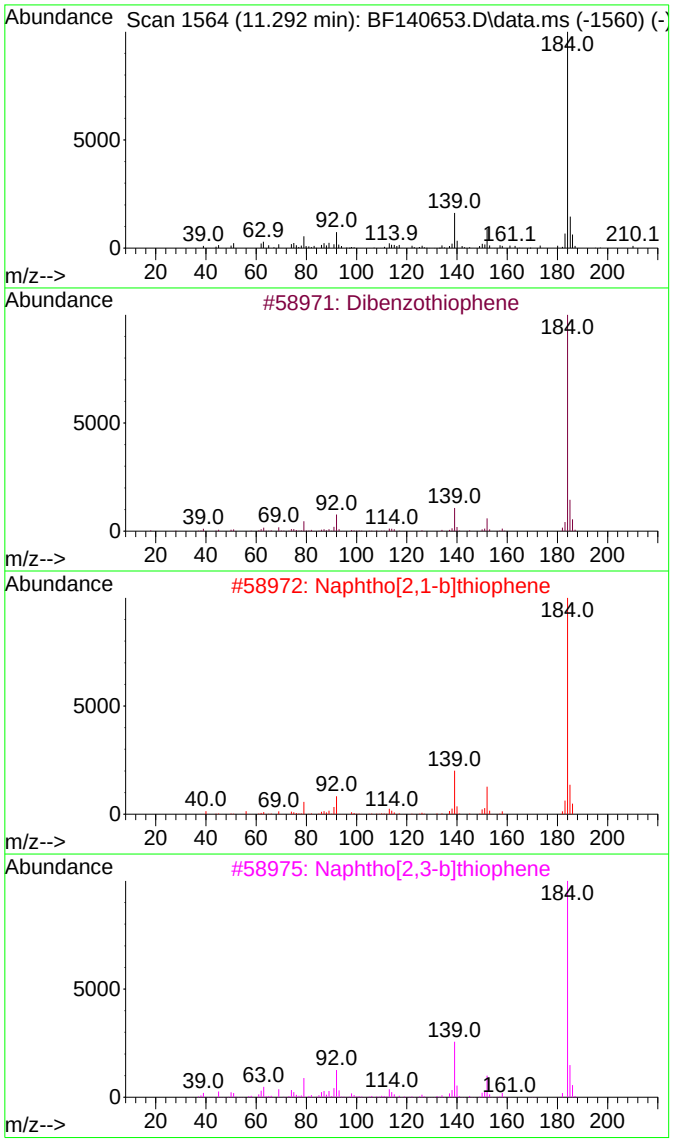
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

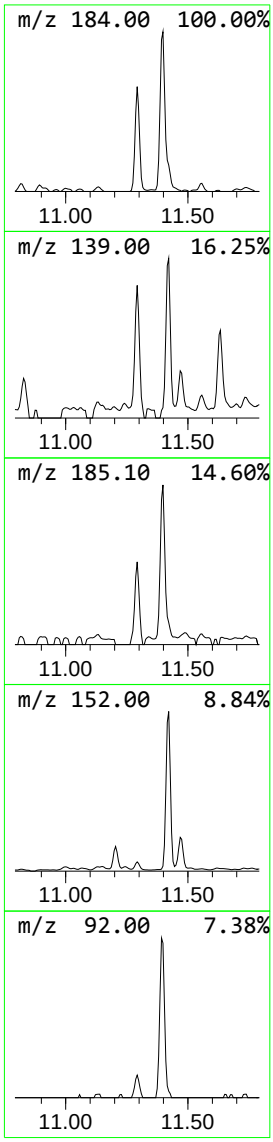
****

Peak Number 2 Dibenzothiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.292	2.39 ng	64038	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	95
2	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	95
3	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	94
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	94
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

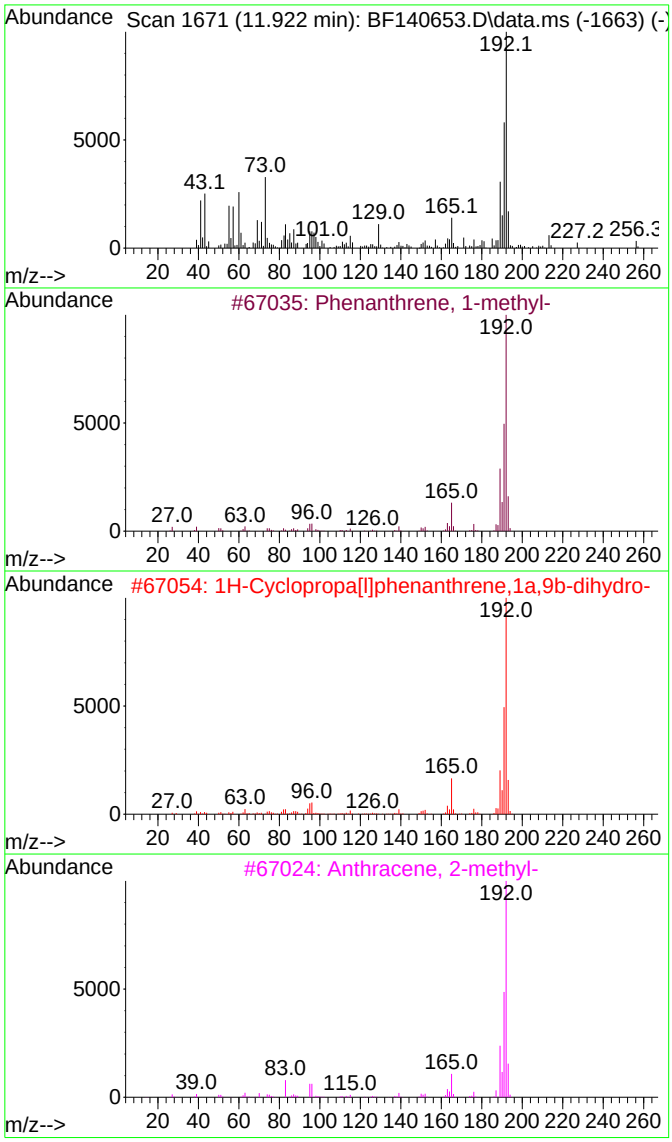
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

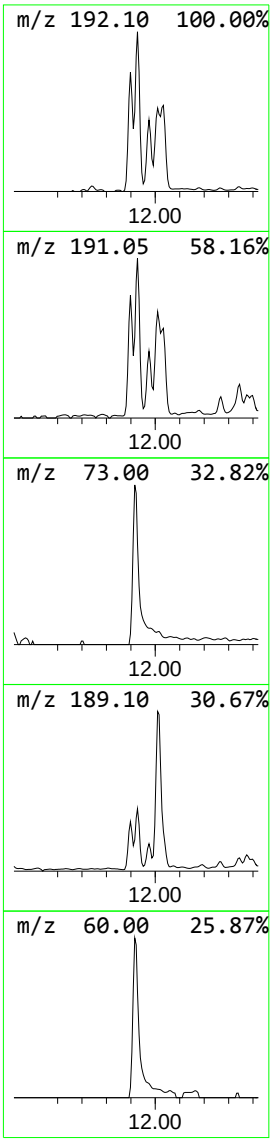
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	10.99 ng	294046	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

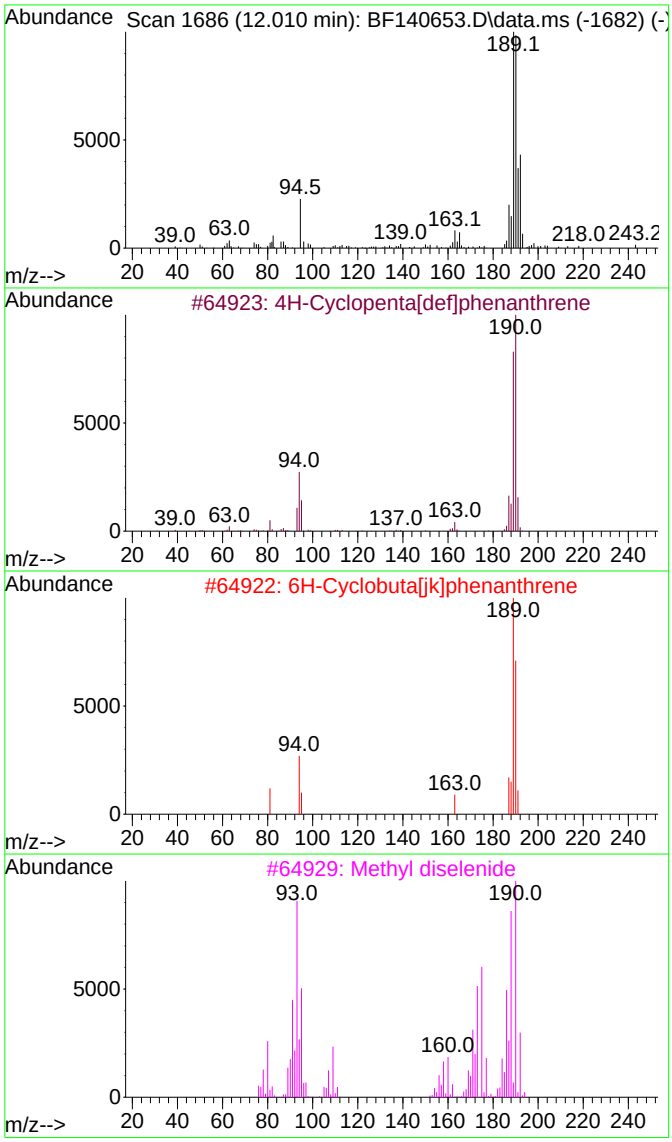
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

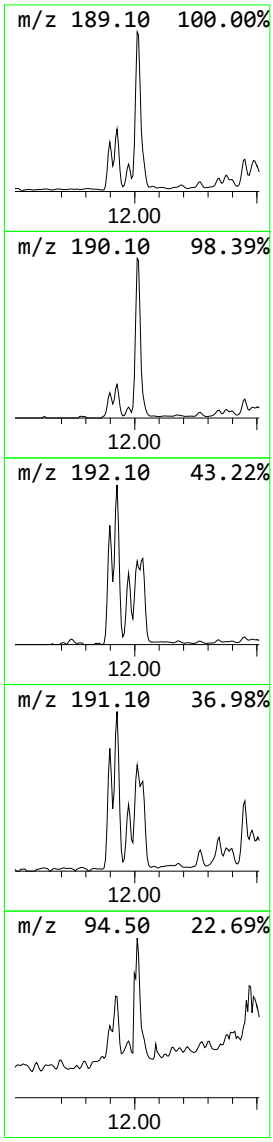
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	6.77 ng	181312	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
5	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	32





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Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
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Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

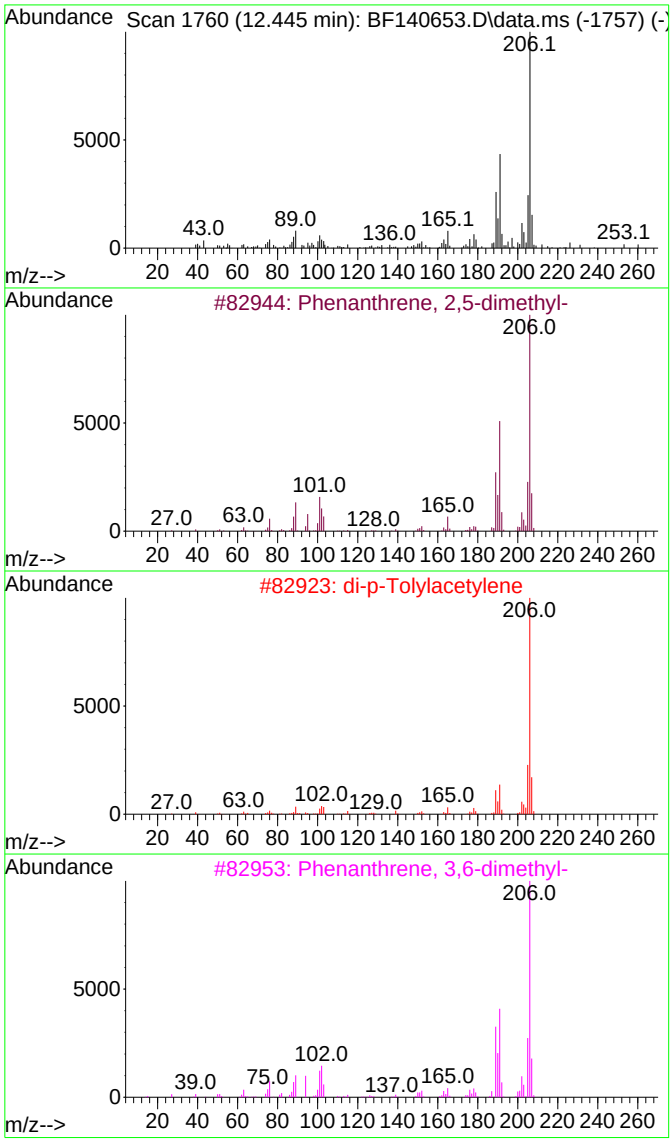
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

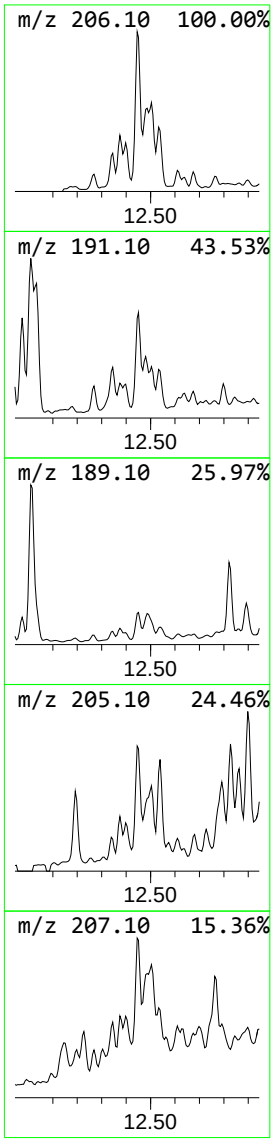
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	2.55 ng	68320	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	91
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	91
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91





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Operator : RC/JU
Sample : P4971-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112224

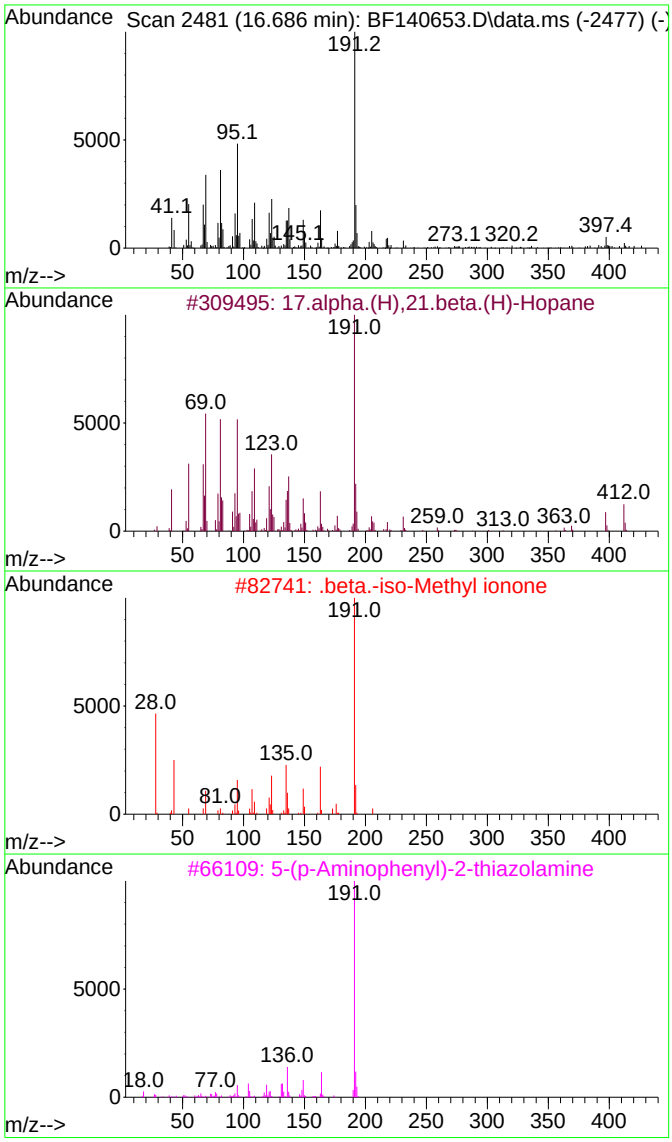
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

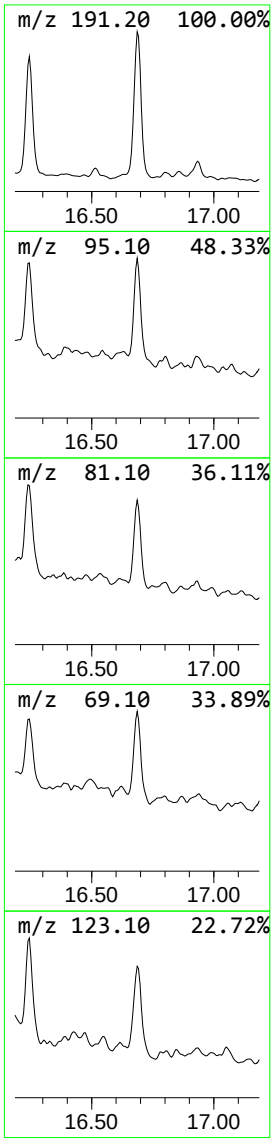
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.686	13.01 ng	311806	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	78
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	46
4	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	43
5	Amberonne (isomer 2)	234	C16H26O	1010470-69-8	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112624\
Data File : BF140653.D
Acq On : 26 Nov 2024 20:11
Operator : RC/JU
Sample : P4971-01
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Instrument :
BNA_F
ClientSampleId :
CL-02-112224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzophenone	10.616	9.1	ng	257828	3	9.904	565991	20.0
Dibenzothiophene	11.292	2.4	ng	64038	4	11.398	535284	20.0
Phenanthrene, 1...	11.922	11.0	ng	294046	4	11.398	535284	20.0
4H-Cyclopenta[d...	12.010	6.8	ng	181312	4	11.398	535284	20.0
Phenanthrene, 2...	12.445	2.5	ng	68320	4	11.398	535284	20.0
17.alpha.(H),21...	16.686	13.0	ng	311806	6	15.539	479390	20.0