LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	19	rVB2	13332	23038	2.81%	0.204%
2	5.010	493	497	505	rBV	100730	109186	13.30%	0.967%
3	5.428	564	568	590	rBV	842606	790244	96.26%	6.999%
4	6.434	735	739	756	rBV	819622	754434	91.90%	6.682%
5	6.781	795	798	802	rBV	388471	316105	38.50%	2.800%
6	7.345	890	894	897	rBV	558419	481606	58.66%	4.265%
7	8.057	1012	1015	1018	rBV	434595	372333	45.35%	3.298%
8	8.081	1018	1019	1033	rVB2	29943	31389	3.82%	0.278%
9	8.775	1134	1137	1144	rVV	8633	9508	1.16%	0.084%
10	8.869	1147	1153	1160	rVB3	7485	12060	1.47%	0.107%
11	9.134	1194	1198	1202	rBV	978692	804996	98.05%	7.129%
12	9.539	1265	1267	1273	rVB	13958	13306	1.62%	0.118%
13	9.675	1287	1290	1294	rBV	73754	67745	8.25%	0.600%
14	9.816	1310	1314	1317	rBV	459139	355420	43.29%	3.148%
15	9.845	1317	1319	1325	rVB	24693	23087	2.81%	0.204%
16	10.022	1345	1349	1353	rBV2	12326	14796	1.80%	0.131%
17	10.369	1405	1408	1414	rVB	22043	26934	3.28%	0.239%
18	10.481	1424	1427	1432	rVB4	11659	15692	1.91%	0.139%
19	10.610	1445	1449	1459	rBV	514573	458362	55.83%	4.059%
20	10.739	1466	1471	1474	rVB4	11526	16774	2.04%	0.149%
21	10.910	1497	1500	1503	rBV5	9458	11089	1.35%	0.098%
22	11.069	1524	1527	1533	rVB3	8983	10637	1.30%	0.094%
23	11.116	1533	1535	1539	rVB	13639	12600	1.53%	0.112%
24	11.169	1539	1544	1547	rBV4	7706	10822	1.32%	0.096%
25	11.204	1547	1550	1554	rVB	17382	17011	2.07%	0.151%
26	11.263	1557	1560	1564	rBV4	13662	15160	1.85%	0.134%
27	11.310	1564	1568	1570	rBV	434726	374192	45.58%	3.314%
28	11.333	1570	1572	1575	rVV	308065	233676	28.46%	2.070%
29	11.386	1578	1581	1584	rVB	97093	77031	9.38%	0.682%
30	11.422	1584	1587	1590	rBV2	24799	25005	3.05%	0.221%
31	11.551	1602	1609	1612	rBV2	40677	57712	7.03%	0.511%
32	11.651	1622	1626	1629	rVB3	7573	12940	1.58%	0.115%
33	11.775	1644	1647	1650	rBV5	16419	20945	2.55%	0.185%
34	11.816	1650	1654	1656	rVV	55540	55211	6.73%	0.489%
35	11.845	1656	1659	1663	rVV	202105	207421	25.27%	1.837%
36	11.892	1665	1667	1670	rVV	31048	27572	3.36%	0.244%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.928	1670	1673	1675	rVV	82649	83698	10.20%	0.741%
38	11.951	1675	1677	1682	rVB	37149	35756	4.36%	0.317%
39	12.004	1682	1686	1688	rBV4	11936	16523	2.01%	0.146%
40	12.110	1702	1704	1707	rBV	34971	28972	3.53%	0.257%
41	12.145	1707	1710	1713	rVB	31640	30706	3.74%	0.272%
42	12.263	1727	1730	1733	rBV3	10361	9868	1.20%	0.087%
43	12.292	1733	1735	1737	rVB	17396	12099	1.47%	0.107%
44	12.316	1737	1739	1742	rVB3	13454	10865	1.32%	0.096%
45	12.363	1744	1747	1750	rBV	34671	38013	4.63%	0.337%
46	12.404	1750	1754	1756	rBV3	21764	28355	3.45%	0.251%
47	12.427	1756	1758	1760	rVB3	14473	10881	1.33%	0.096%
48	12.457	1760	1763	1767	rBV3	34378	42175	5.14%	0.374%
49	12.533	1770	1776	1778	rBV	562815	512290	62.40%	4.537%
50	12.627	1789	1792	1796	rBV2	46912	53092	6.47%	0.470%
51	12.763	1809	1815	1820	rVB	547700	526574	64.14%	4.664%
52	12.810	1820	1823	1829	rVB2	25014	26830	3.27%	0.238%
53	12.904	1832	1839	1842	rBV	869872	739166	90.04%	6.546%
54	12.980	1848	1852	1856	rBV3	38449	60089	7.32%	0.532%
55	13.092	1864	1871	1874	rVB	90242	132054	16.09%	1.170%
56	13.157	1880	1882	1885	rBV2	53034	46229	5.63%	0.409%
57	13.198	1885	1889	1891	rVV2	59282	62080	7.56%	0.550%
58	13.286	1902	1904	1907	rBV	61023	56379	6.87%	0.499%
59	13.322	1907	1910	1913	rVV	47694	45686	5.56%	0.405%
60	13.604	1956	1958	1962	rVB	57541	56639	6.90%	0.502%
61	13.663	1966	1968	1970	rVB2	24523	17427	2.12%	0.154%
62	13.716	1975	1977	1980	rVB	38634	33281	4.05%	0.295%
63	13.769	1984	1986	1987	rBV	57090	43443	5.29%	0.385%
64	13.816	1992	1994	1998	rVB	50309	48404	5.90%	0.429%
65	13.969	2013	2020	2023	rBV2	537839	820965	100.00%	7.271%
66	13.998	2023	2025	2032	rVB	251615	235049	28.63%	2.082%
67	15.021	2196	2199	2202	rBV	265636	370329	45.11%	3.280%
68	15.333	2248	2252	2257	rVB	181093	234412	28.55%	2.076%
69	15.398	2259	2263	2269	rVB	208841	264416	32.21%	2.342%
70	15.457	2270	2273	2277	rBV2	221552	285934	34.83%	2.532%
71	16.980	2527	2532	2541	rVB2	108675	223056	27.17%	1.975%
72	17.439	2605	2610	2620	rVB	89150	183496	22.35%	1.625%

Sum of corrected areas: 11291270

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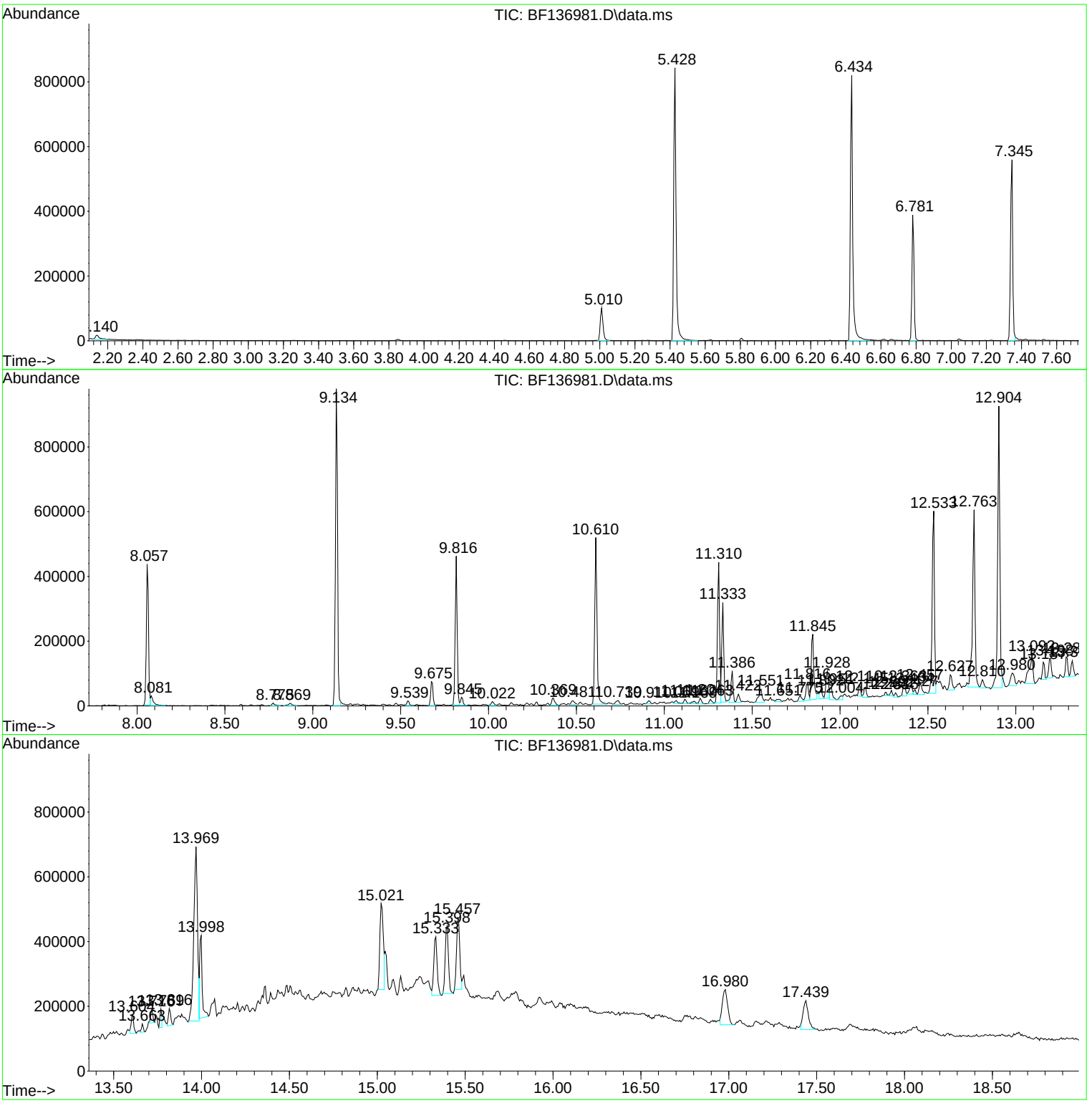
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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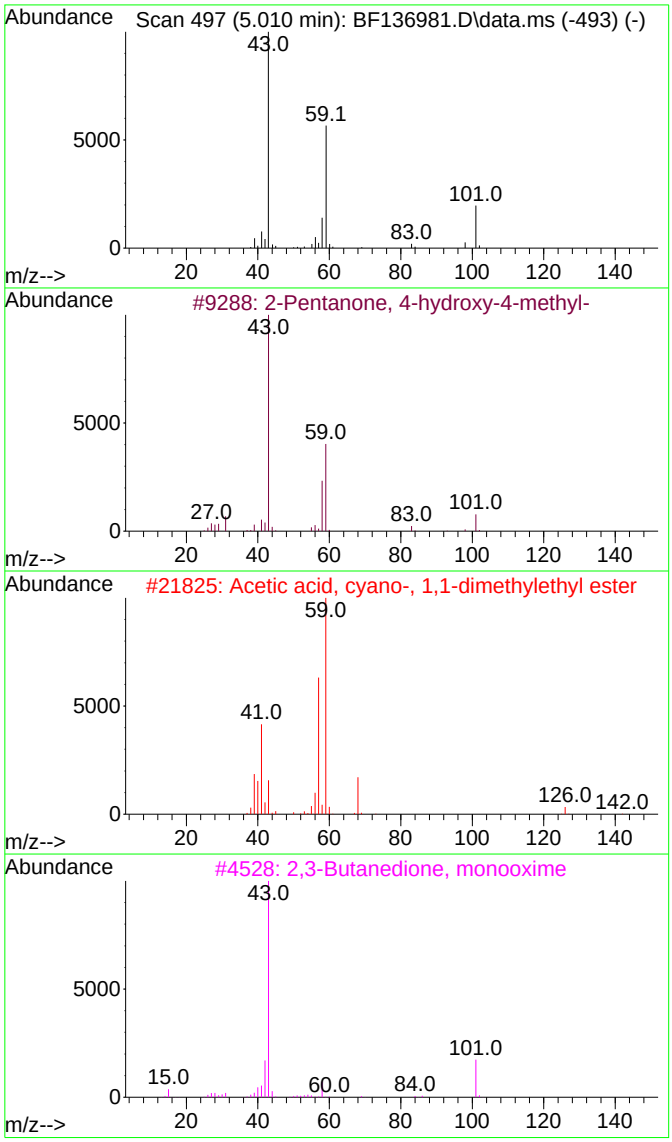
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

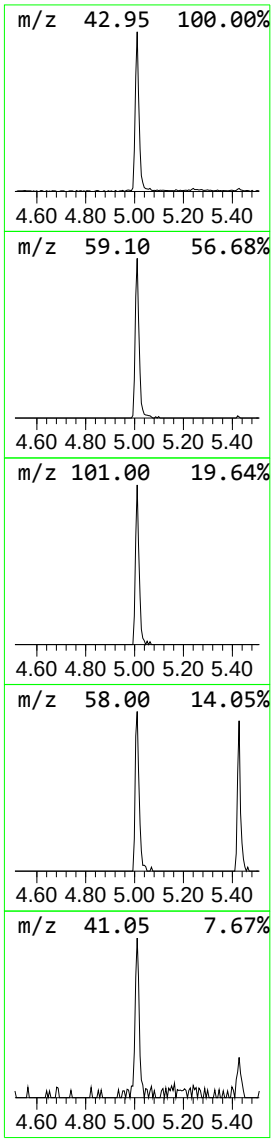
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	6.91 ng	109186	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
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Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

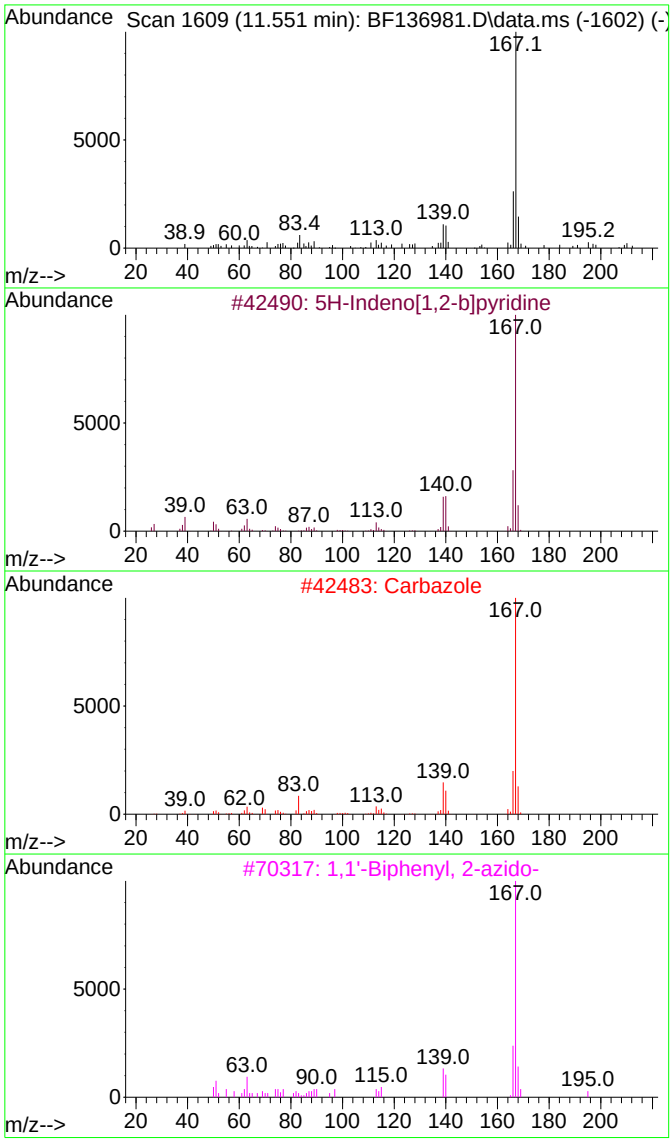
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

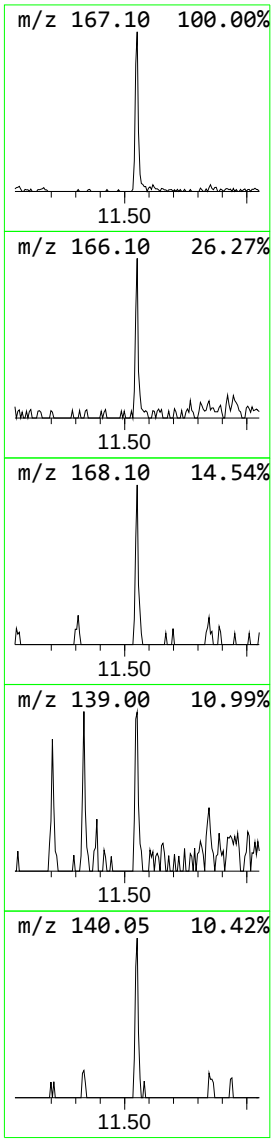
****

Peak Number 2 5H-Indeno[1,2-b]pyridine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.551	3.08 ng	57712	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	90
2	Carbazole	167	C12H9N	000086-74-8	87
3	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	87
4	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	86
5	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	86





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Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

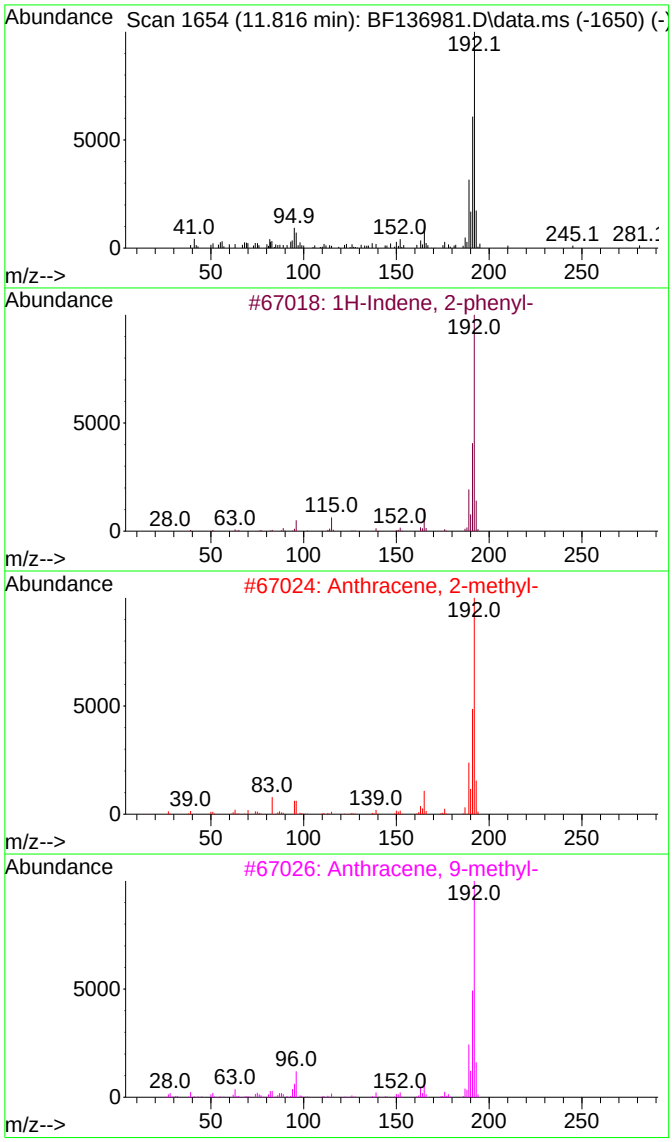
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

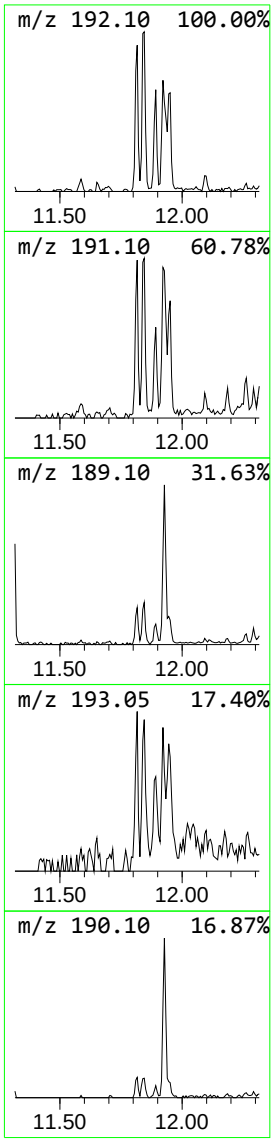
****

Peak Number 3 1H-Indene, 2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	2.95 ng	55211	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	87
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	87





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Data File : BF136981.D
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Instrument :
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ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

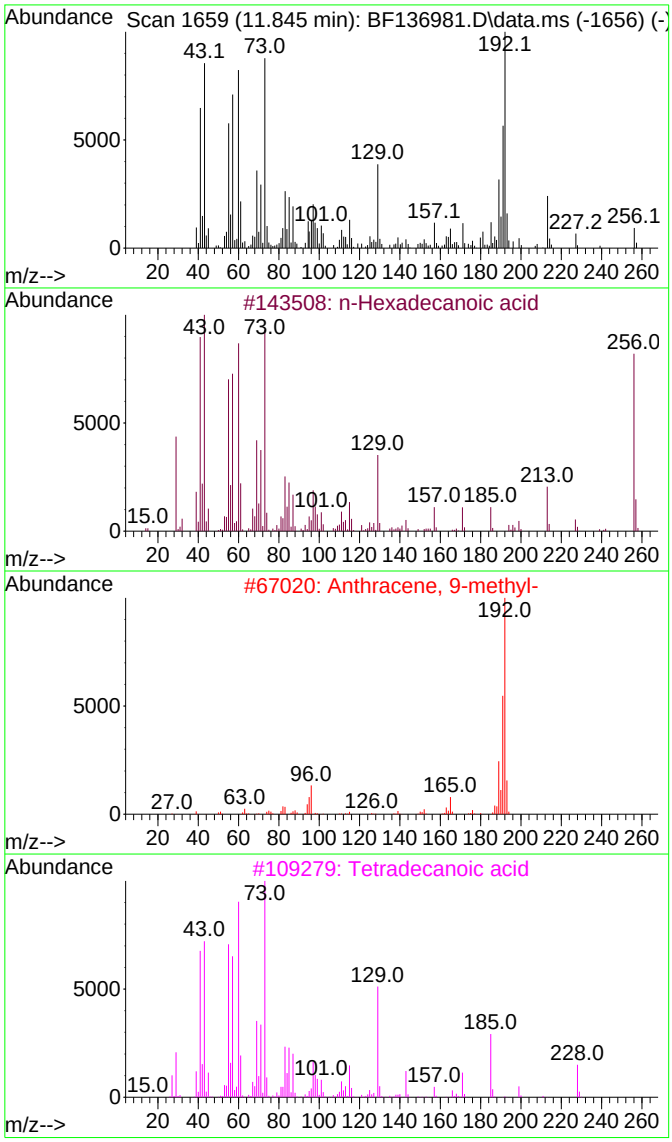
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

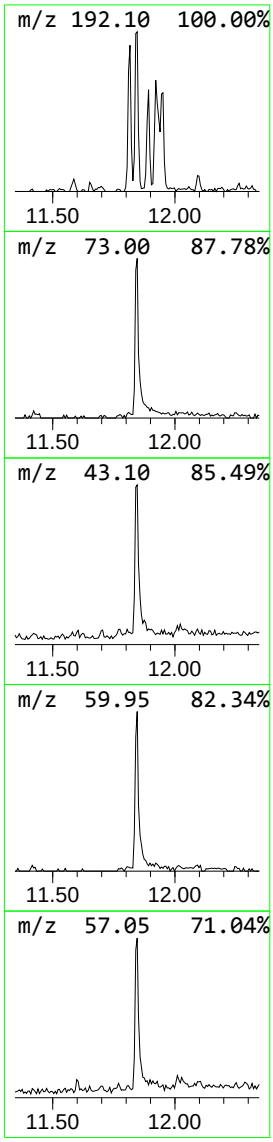
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	11.09 ng	207421	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
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Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

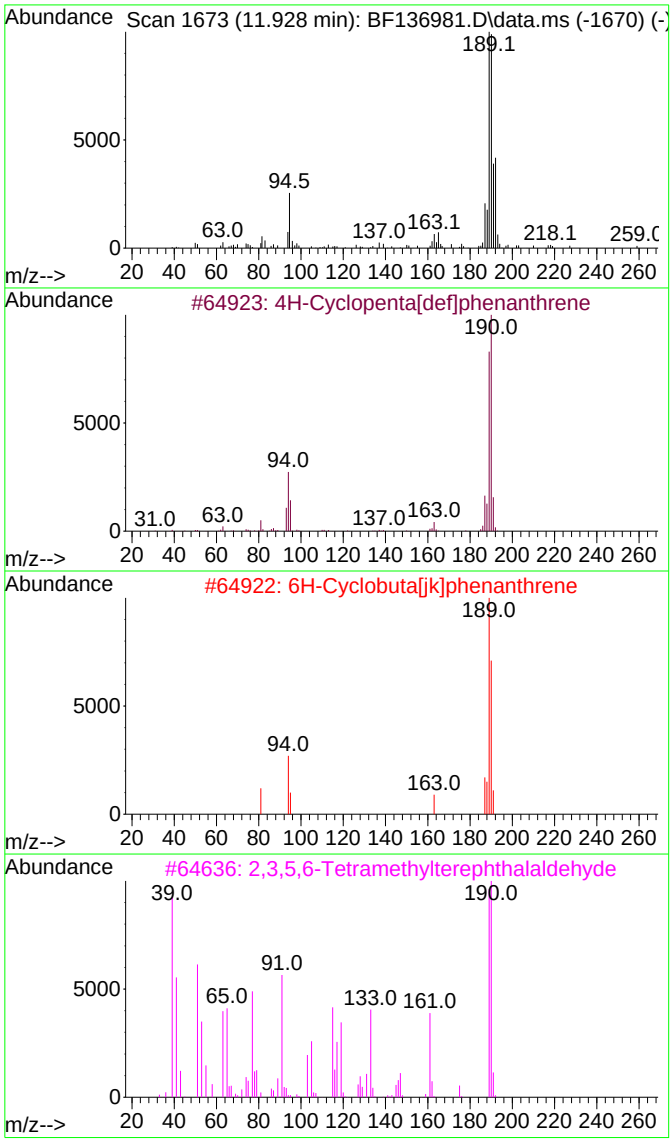
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

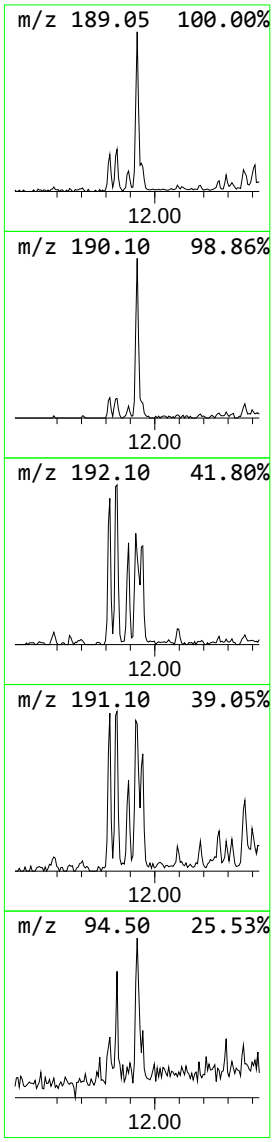
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	4.47 ng	83698	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

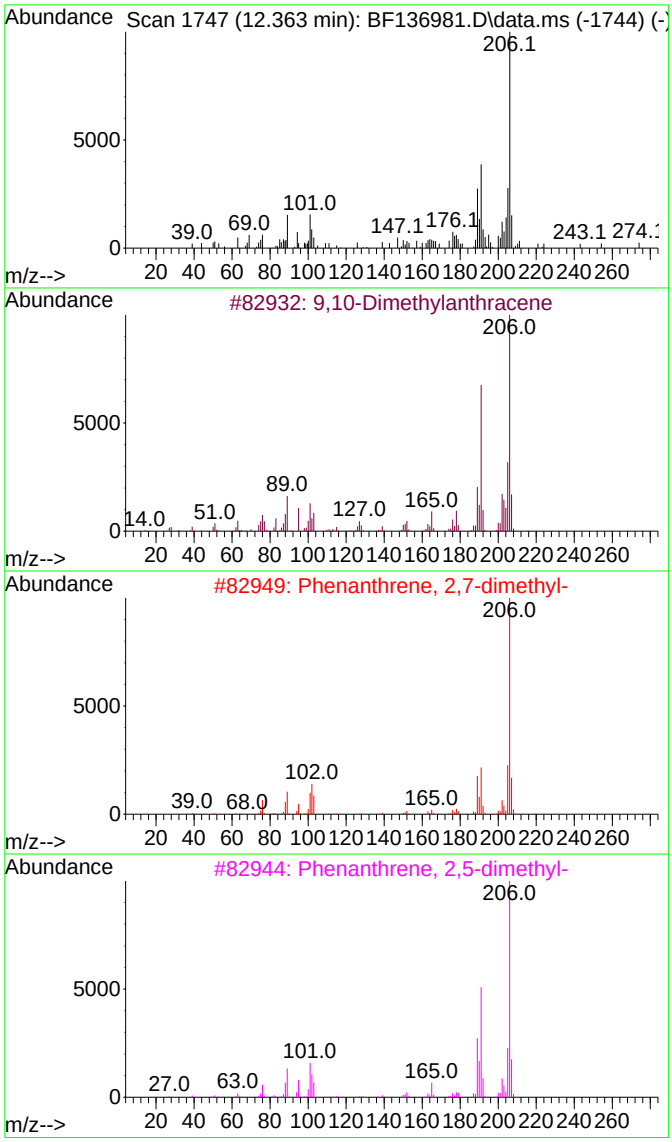
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

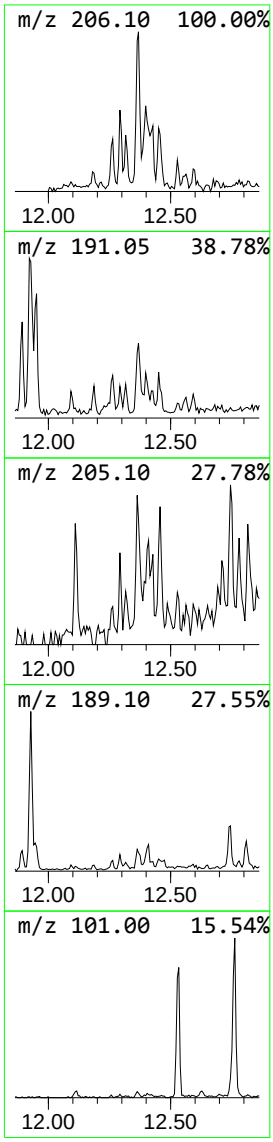
****

Peak Number 6 9,10-Dimethylanthracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	2.03 ng	38013	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
2	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	93
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

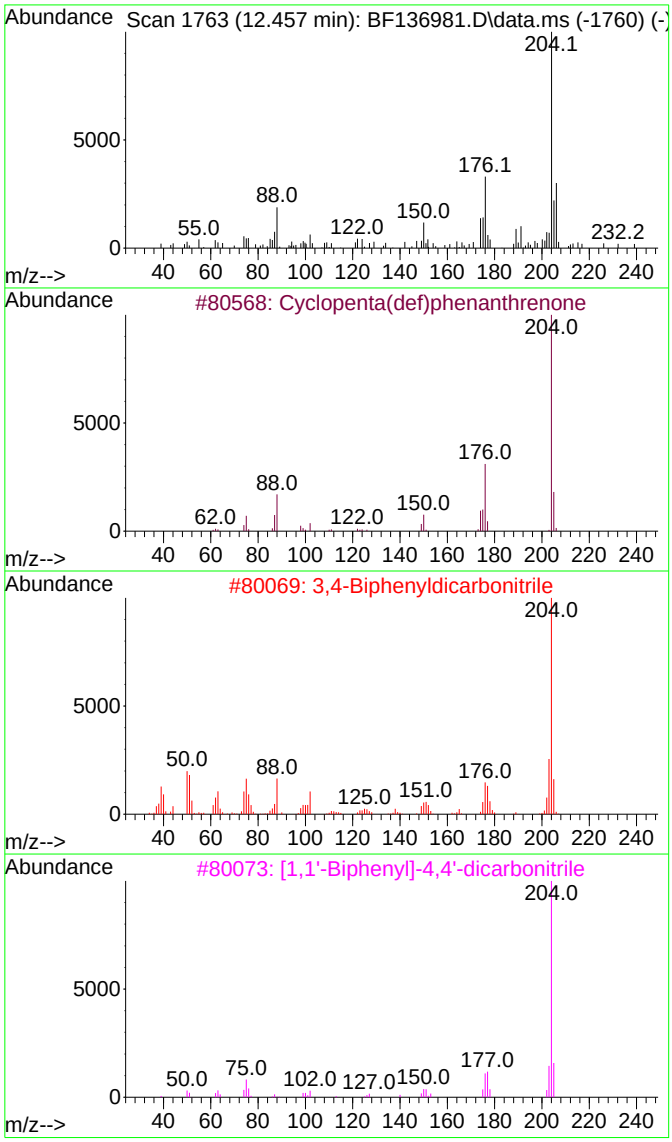
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

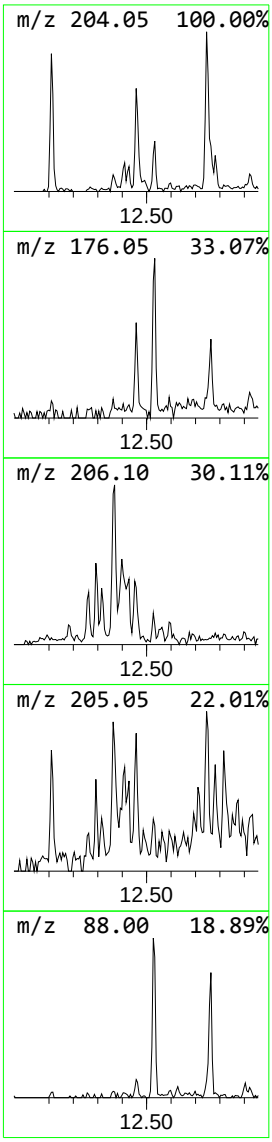
****

Peak Number 7 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	2.25 ng	42175	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	91
2	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	53
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	46
5	Quinoline, 8-methoxy-5-nitro-	204	C10H8N2O3	1000298-88-7	46





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Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

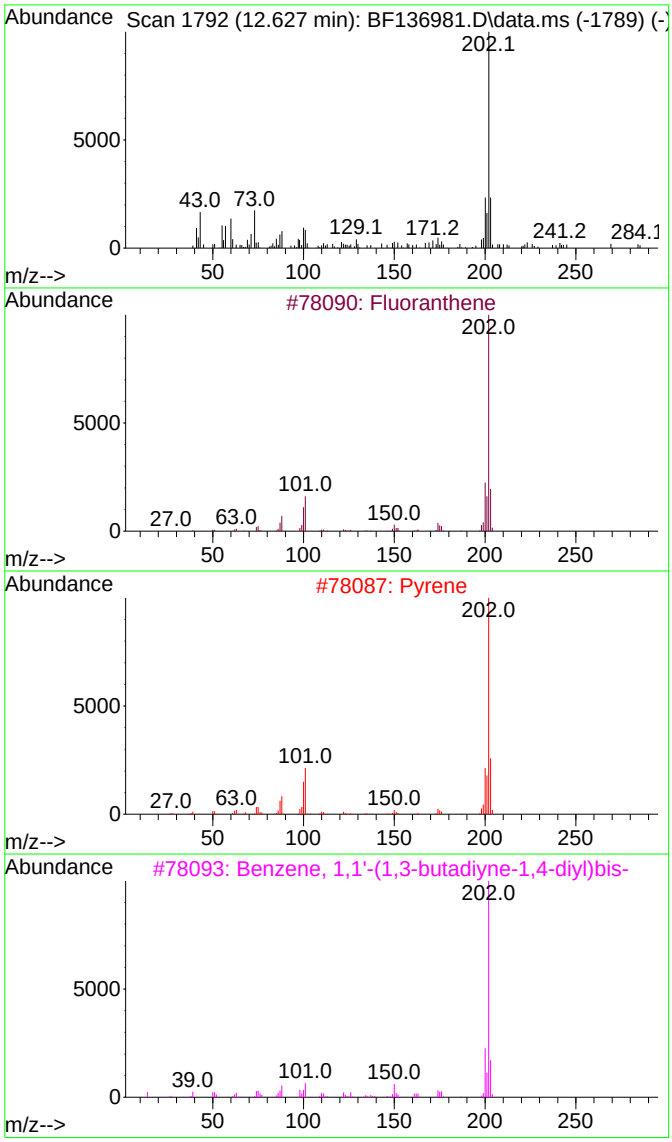
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

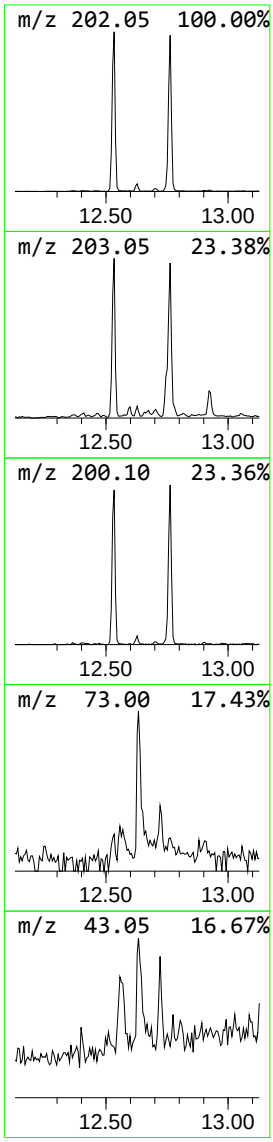
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	2.84 ng	53092	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	86
2	Pyrene	202	C16H10	000129-00-0	70
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	Methyl 3-indolepropionate, TMS d...	275	C15H21NO2Si	056196-72-6	50
5	Anthracene, 9-(2-nitroethenyl)-	249	C16H11NO2	058349-77-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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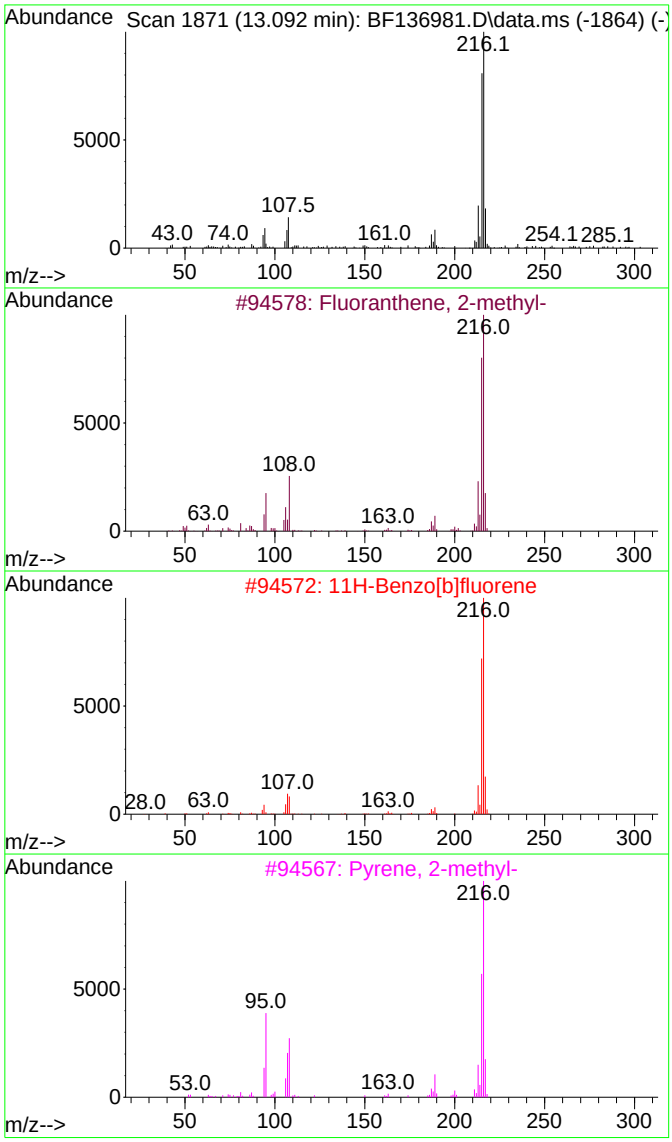
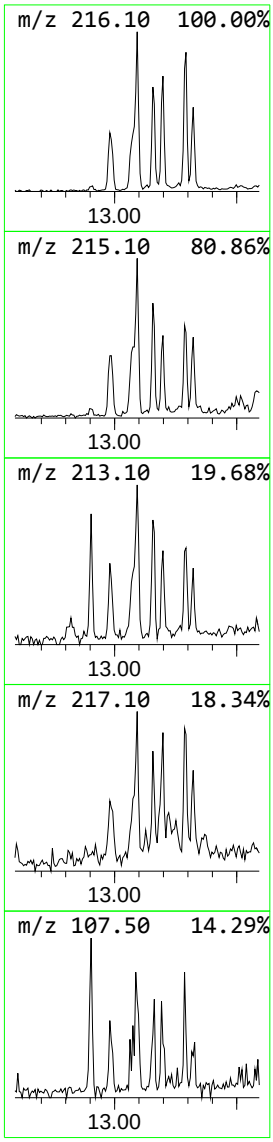
Peak Number 9 Fluoranthene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.092	3.22 ng	132054	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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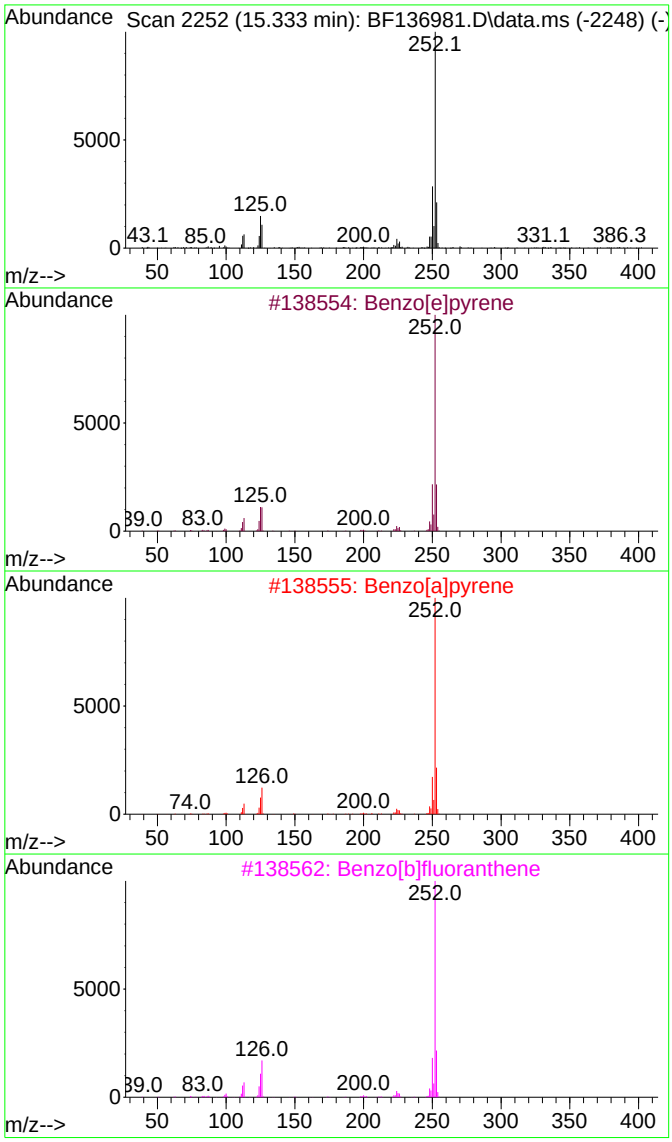
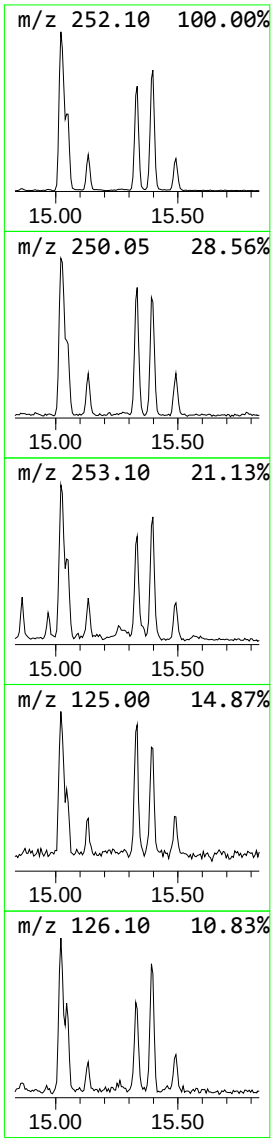
Peak Number 10 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	16.40 ng	234412	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136981.D
Acq On : 05 Jan 2024 17:57
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.010	6.9	ng	109186	1	6.781	316105	20.0
5H-Indeno[1,2-b...	11.551	3.1	ng	57712	4	11.310	374192	20.0
1H-Indene, 2-ph...	11.816	3.0	ng	55211	4	11.310	374192	20.0
n-Hexadecanoic ...	11.845	11.1	ng	207421	4	11.310	374192	20.0
4H-Cyclopenta[d...	11.928	4.5	ng	83698	4	11.310	374192	20.0
9,10-Dimethylan...	12.363	2.0	ng	38013	4	11.310	374192	20.0
Cyclopenta(def)...	12.457	2.3	ng	42175	4	11.310	374192	20.0
Benzene, 1,1'-(...	12.628	2.8	ng	53092	4	11.310	374192	20.0
Fluoranthene, 2...	13.092	3.2	ng	132054	5	13.969	820965	20.0
Benzo[e]pyrene	15.333	16.4	ng	234412	6	15.463	285934	20.0