LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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: BF136964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	492	495	503	rBV	79937	84799	13.01%	0.972%
2	5.422	564	567	583	rBV	652315	626893	96.21%	7.185%
3	6.434	735	739	751	rBV	675898	624750	95.88%	7.161%
4	6.781	795	798	802	rBV	305440	242576	37.23%	2.780%
5	7.345	890	894	897	rBV	460854	381522	58.55%	4.373%
6	8.057	1012	1015	1018	rBV	333166	293220	45.00%	3.361%
7	8.081	1018	1019	1029	rVB	23127	23919	3.67%	0.274%
8	9.134	1195	1198	1202	rBV	816987	651606	100.00%	7.468%
9	9.545	1264	1268	1272	rVB	10038	11272	1.73%	0.129%
10	9.681	1287	1291	1294	rBV	55611	51392	7.89%	0.589%
11	9.816	1311	1314	1318	rBV	385723	298123	45.75%	3.417%
12	9.851	1318	1320	1323	rVB	18972	15855	2.43%	0.182%
13	10.022	1345	1349	1353	rBV	8625	10060	1.54%	0.115%
14	10.369	1405	1408	1414	rVB	21143	22741	3.49%	0.261%
15	10.481	1424	1427	1432	rVB5	9537	11998	1.84%	0.138%
16	10.610	1446	1449	1459	rVB	432019	386203	59.27%	4.426%
17	10.739	1466	1471	1475	rVB5	9368	12286	1.89%	0.141%
18	10.922	1498	1502	1504	rBV5	5722	8538	1.31%	0.098%
19	11.116	1533	1535	1539	rVB2	13204	11534	1.77%	0.132%
20	11.169	1539	1544	1548	rBV4	5778	11668	1.79%	0.134%
21	11.204	1548	1550	1557	rVB	14857	14260	2.19%	0.163%
22	11.263	1557	1560	1564	rBV4	10909	11912	1.83%	0.137%
23	11.310	1564	1568	1570	rVV	369917	313887	48.17%	3.598%
24	11.333	1570	1572	1576	rVV	284228	209539	32.16%	2.402%
25	11.386	1578	1581	1584	rVV	83052	64870	9.96%	0.744%
26	11.422	1584	1587	1592	rVB2	19194	21732	3.34%	0.249%
27	11.551	1603	1609	1612	rBV2	30815	39039	5.99%	0.447%
28	11.645	1623	1625	1630	rVB4	8826	11457	1.76%	0.131%
29	11.704	1631	1635	1637	rBV4	6565	8459	1.30%	0.097%
30	11.775	1644	1647	1651	rBV4	13351	18699	2.87%	0.214%
31	11.816	1651	1654	1656	rVV	46851	43813	6.72%	0.502%
32	11.845	1656	1659	1663	rVV	162208	162561	24.95%	1.863%
33	11.892	1665	1667	1670	rVV	26174	25653	3.94%	0.294%
34	11.928	1670	1673	1675	rVV	70161	71879	11.03%	0.824%
35	11.951	1675	1677	1683	rVB2	33984	31362	4.81%	0.359%
36	12.010	1683	1687	1688	rBV4	8799	10558	1.62%	0.121%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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	12.110	1702	1704	1707	rVB	27367	24649	3.78%	0.283%
38	12.145	1707	1710	1715	rVB2	25512	24375	3.74%	0.279%
39	12.263	1727	1730	1733	rBV4	10178	10464	1.61%	0.120%
40	12.369	1745	1748	1750	rBV	32141	32139	4.93%	0.368%
41	12.404	1751	1754	1756	rVV4	20054	23129	3.55%	0.265%
42	12.427	1756	1758	1760	rVB3	12275	9701	1.49%	0.111%
43	12.457	1760	1763	1767	rBV3	31066	36119	5.54%	0.414%
44	12.533	1772	1776	1779	rBV	484079	414473	63.61%	4.750%
45	12.633	1789	1793	1797	rBV2	32983	45363	6.96%	0.520%
46	12.763	1809	1815	1818	rBV	469700	430596	66.08%	4.935%
47	12.816	1821	1824	1828	rBV3	19705	23547	3.61%	0.270%
48	12.904	1833	1839	1846	rVB	684738	608813	93.43%	6.978%
49	12.980	1848	1852	1856	rBV3	34990	58877	9.04%	0.675%
50	13.092	1864	1871	1875	rVB	66816	107814	16.55%	1.236%
51	13.157	1880	1882	1885	rVB	42718	37473	5.75%	0.429%
52	13.198	1885	1889	1892	rBV2	59316	65702	10.08%	0.753%
53	13.292	1902	1905	1907	rBV	58939	46906	7.20%	0.538%
54	13.322	1907	1910	1914	rVV	38112	36079	5.54%	0.414%
55	13.610	1956	1959	1963	rVB	41692	43893	6.74%	0.503%
56	13.716	1975	1977	1980	rVV	31516	26449	4.06%	0.303%
57	13.769	1984	1986	1988	rBV	43807	40099	6.15%	0.460%
58	13.822	1992	1995	1997	rVB	36742	36168	5.55%	0.415%
59	13.969	2013	2020	2023	rBV2	406696	647900	99.43%	7.426%
60	13.998	2023	2025	2029	rVV	203556	193537	29.70%	2.218%
61	14.063	2033	2036	2042	rVB3	54331	96243	14.77%	1.103%
62	15.021	2196	2199	2202	rBV	167122	227584	34.93%	2.608%
63	15.327	2248	2251	2257	rVB	121623	157242	24.13%	1.802%
64	15.398	2259	2263	2269	rBV	144731	182313	27.98%	2.090%
65	15.457	2270	2273	2277	rBV	150714	196658	30.18%	2.254%

Sum of corrected areas: 8724940

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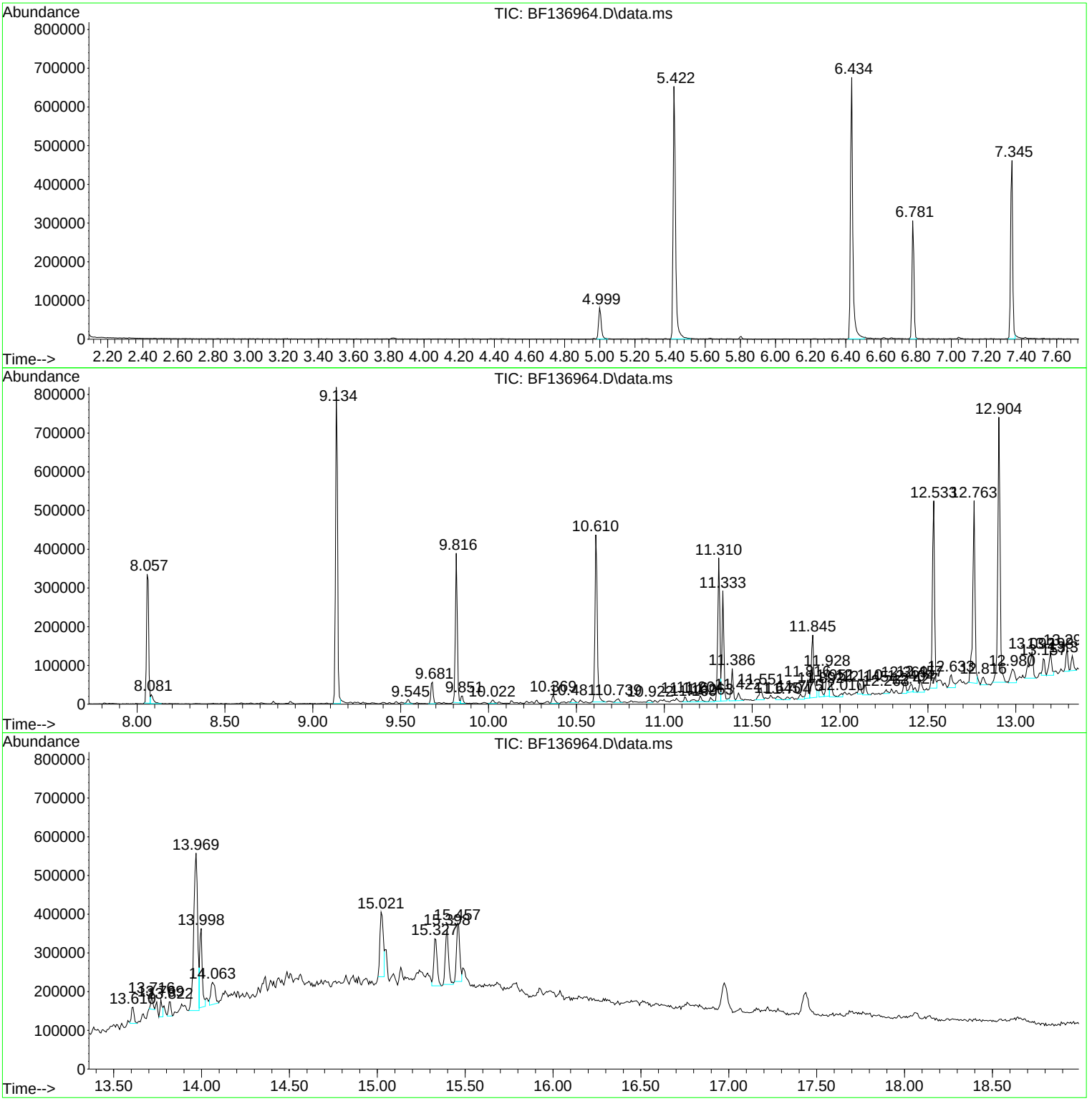
Instrument :
BNA_F
ClientSampleId :
MR-300-0-2

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
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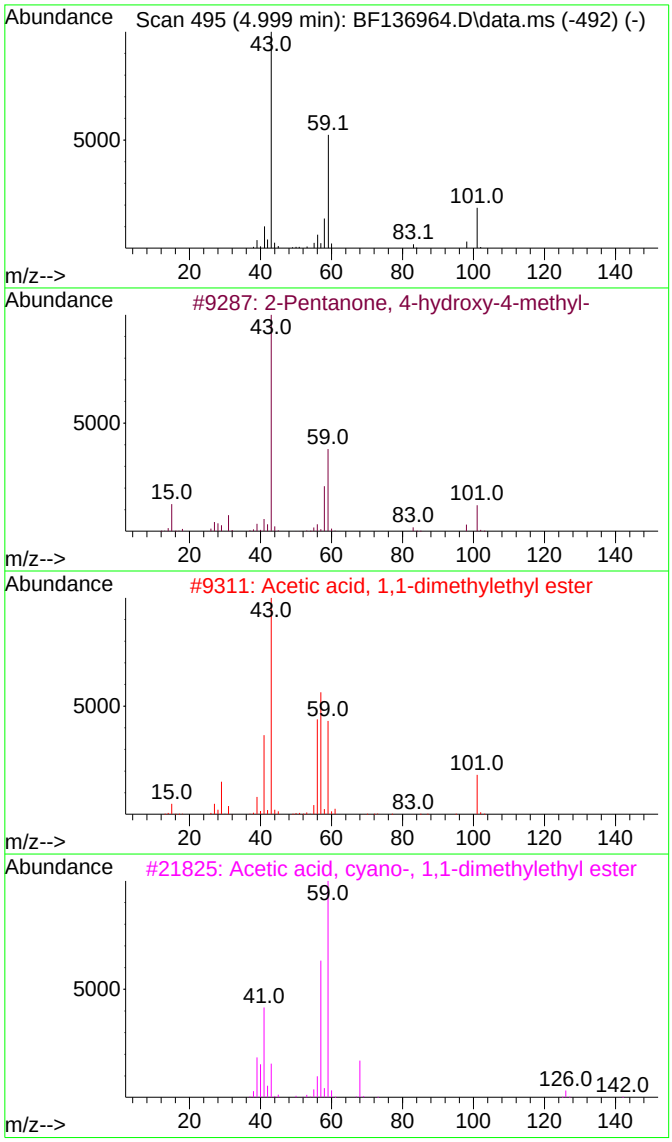
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

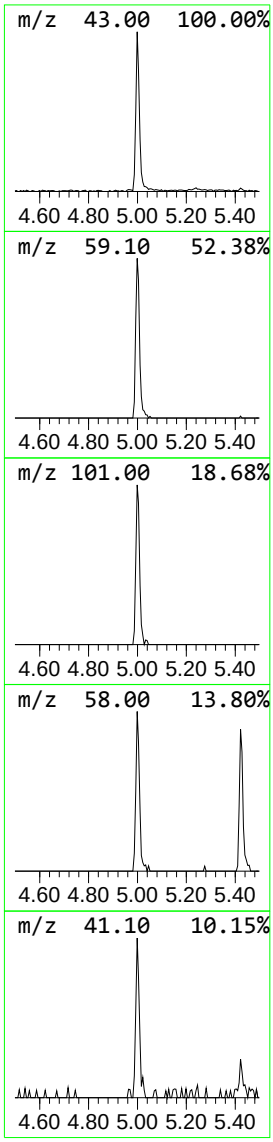
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	6.99 ng	84799	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
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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

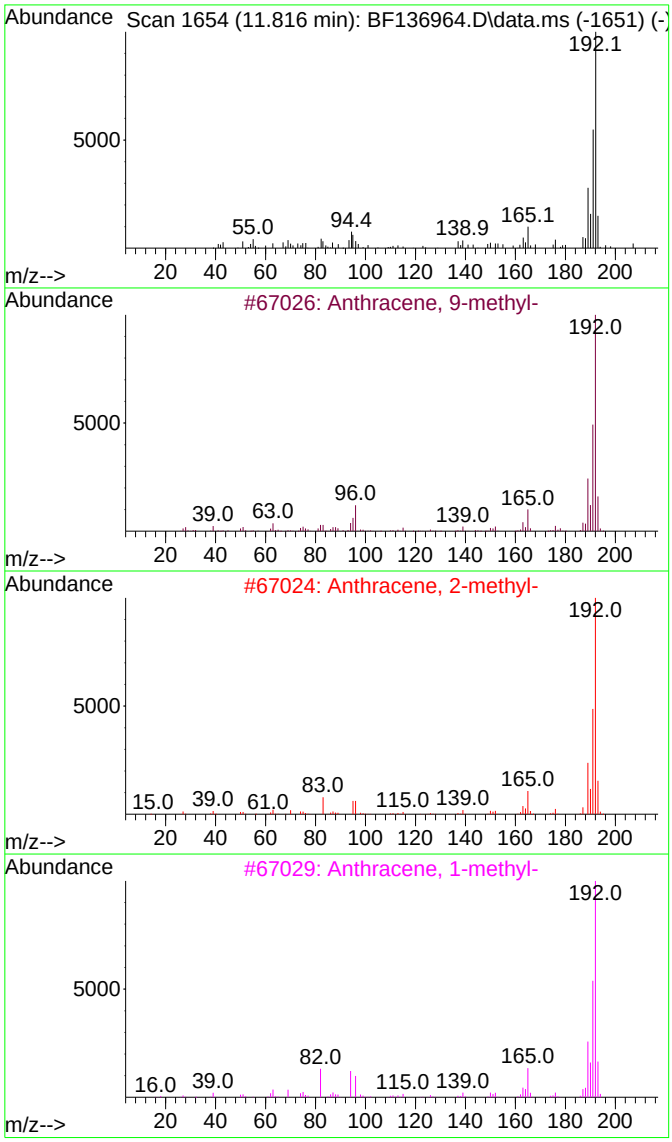
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

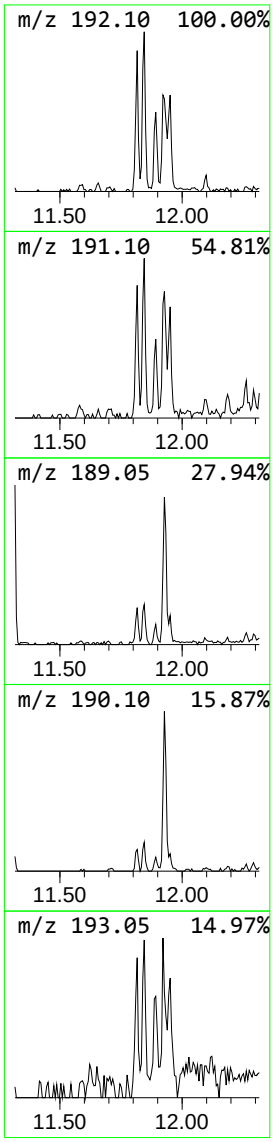
****

Peak Number 3 Anthracene, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	2.79 ng	43813	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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

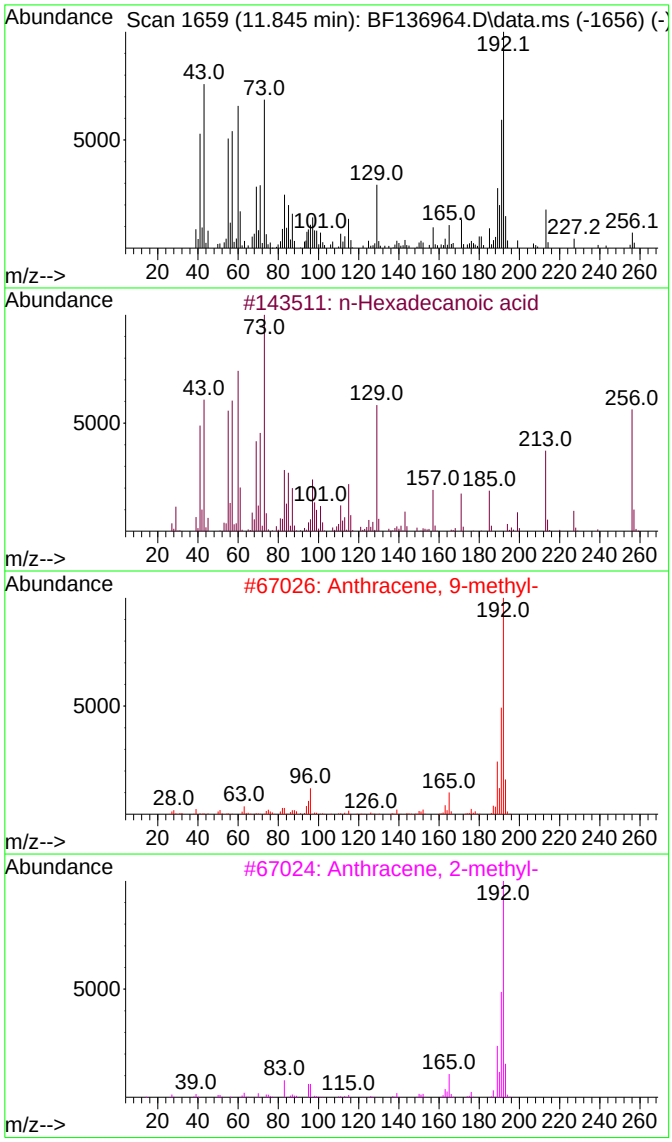
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

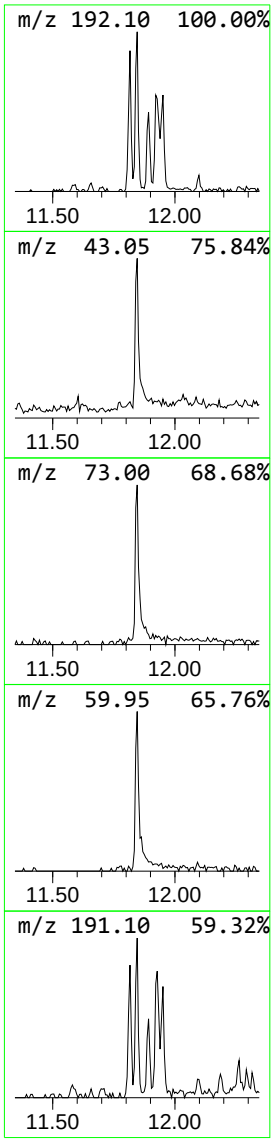
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	10.36 ng	162561	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
3	Anthracene, 2-methyl-	192	C15H12	002531-84-2	89
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	89
5	Tridecanoic acid	214	C13H26O2	000638-53-9	66





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

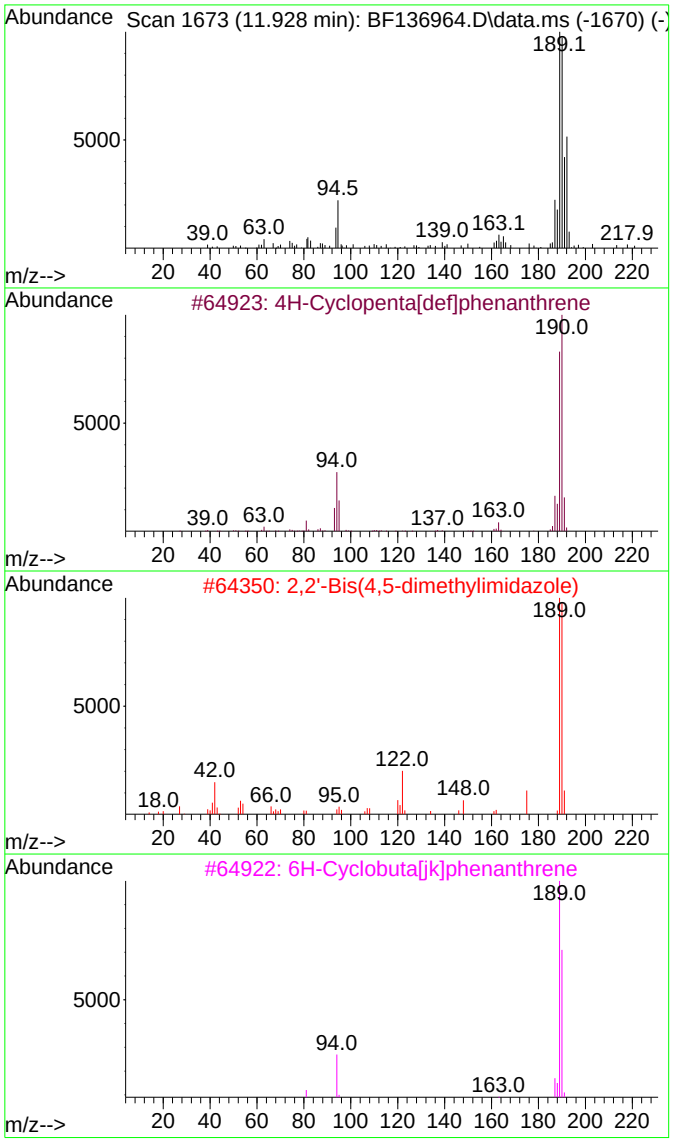
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

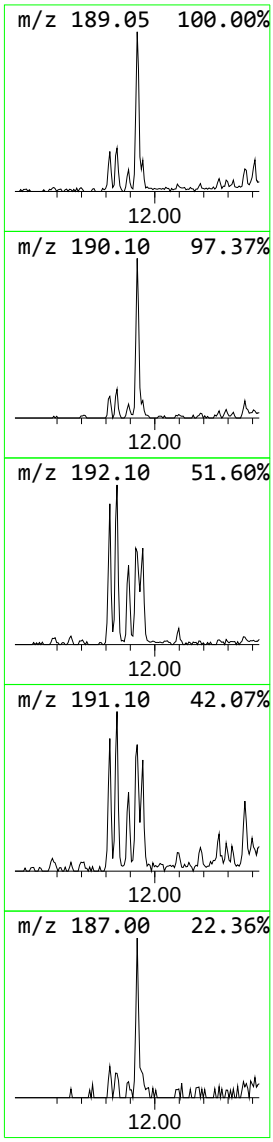
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	4.58 ng	71879	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	Methyl diselenide	190	C2H6Se2	007101-31-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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

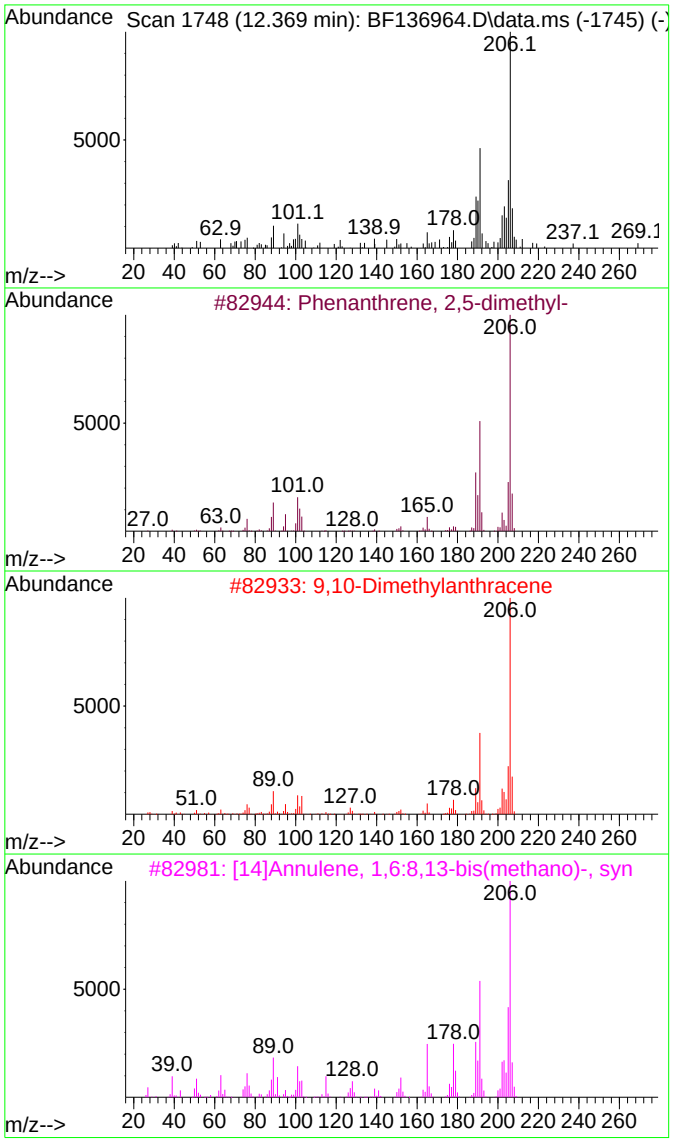
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

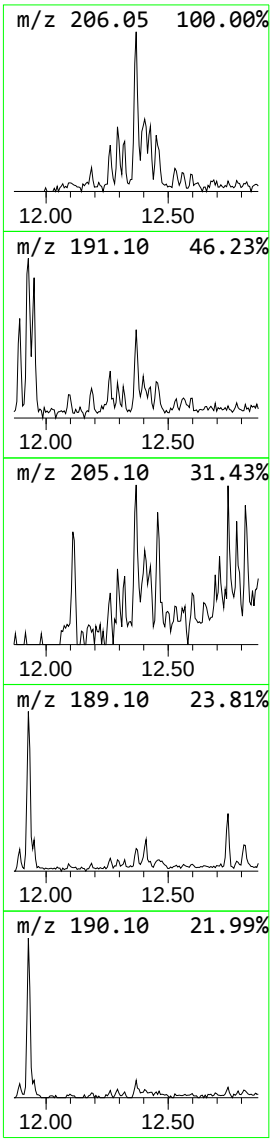
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	2.05 ng	32139	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
3	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	87
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	83
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

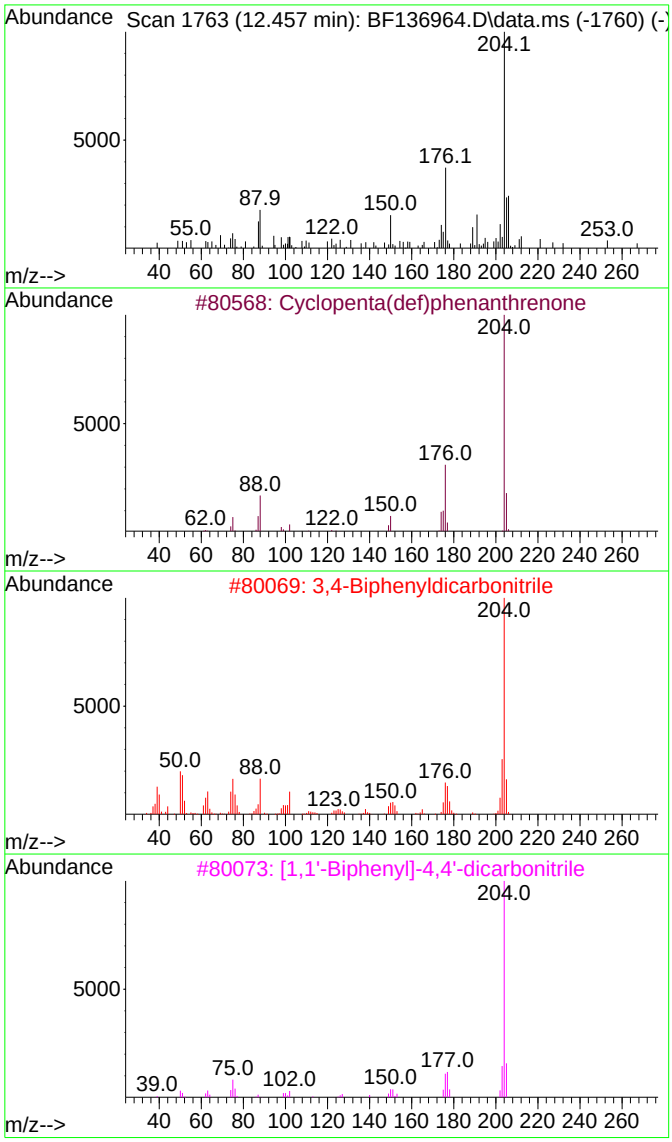
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

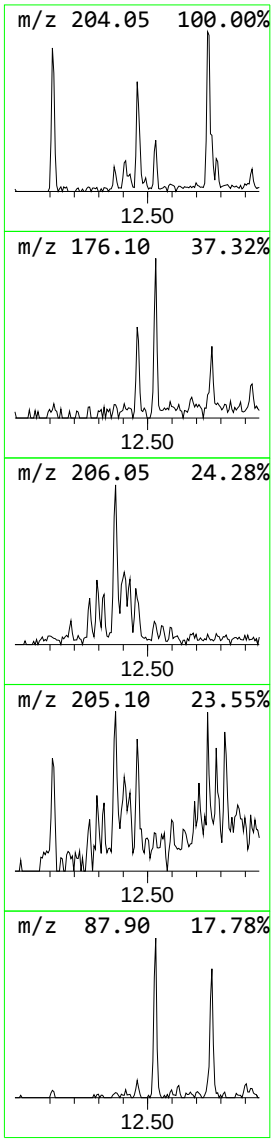
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopenta(def)phenanthrenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	2.30 ng	36119	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	62
2	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	50
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47
4	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	46
5	[1,2,4]Triazolo[5,1-b]quinazolin...	204	C10H12N4O	1000337-56-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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

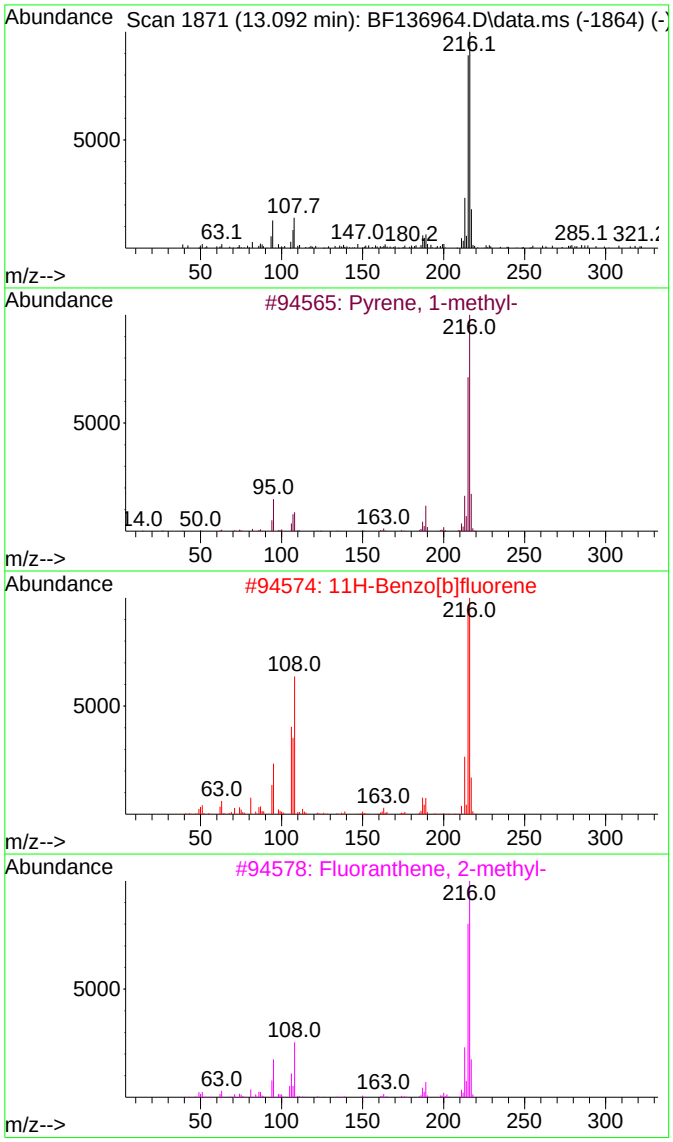
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

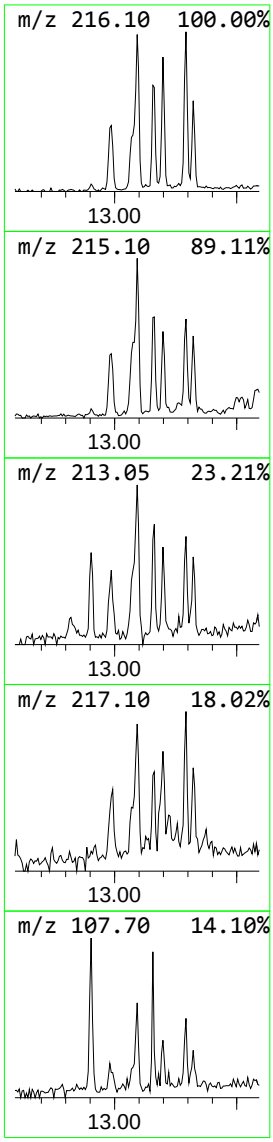
****

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.092	3.33 ng	107814	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





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Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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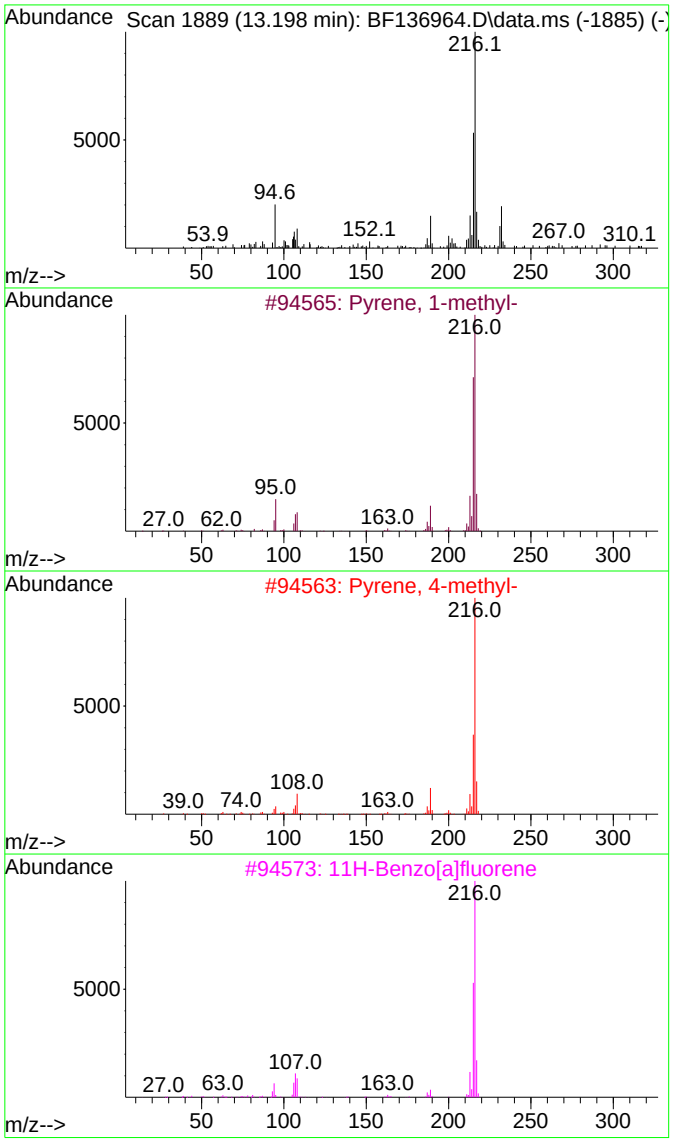
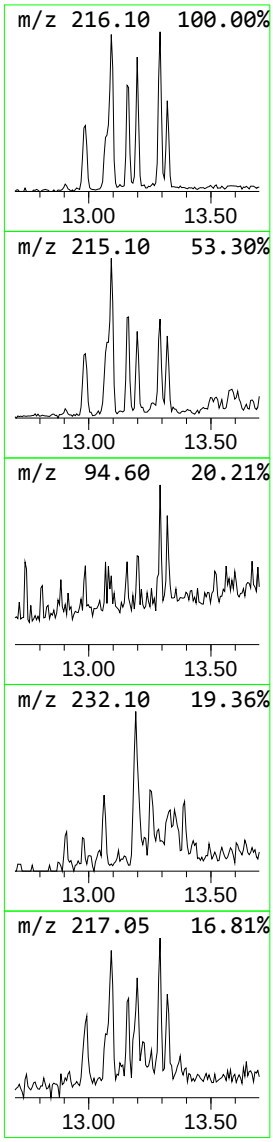
Peak Number 10 Pyrene, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.198	2.03 ng	65702	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	64
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	62
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	58
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	53





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Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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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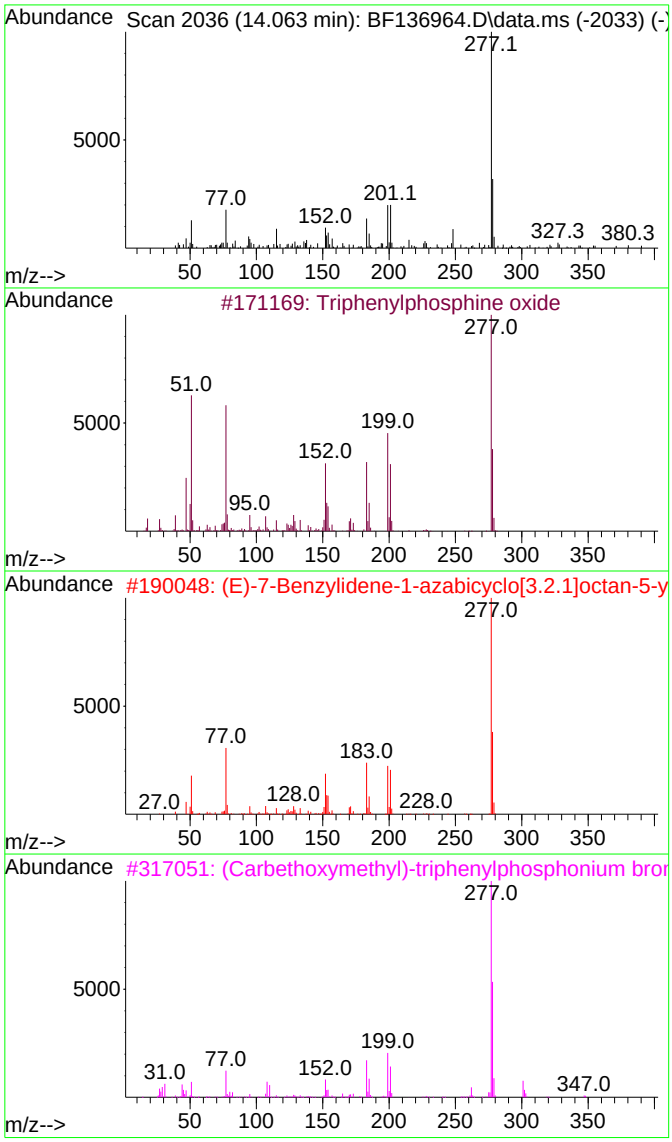
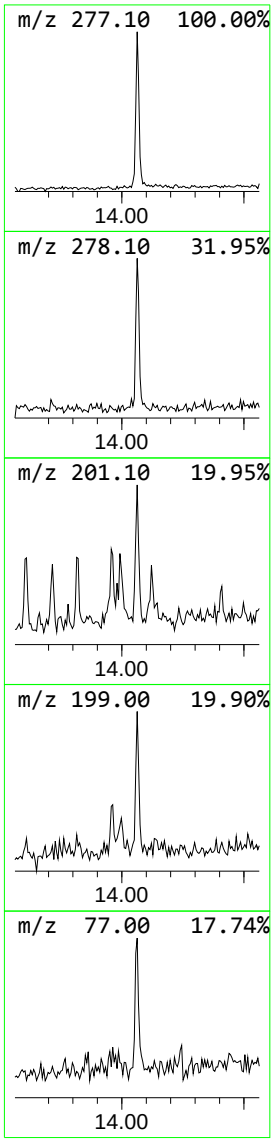
Peak Number 11 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	2.97 ng	96243	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	50
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38
5	5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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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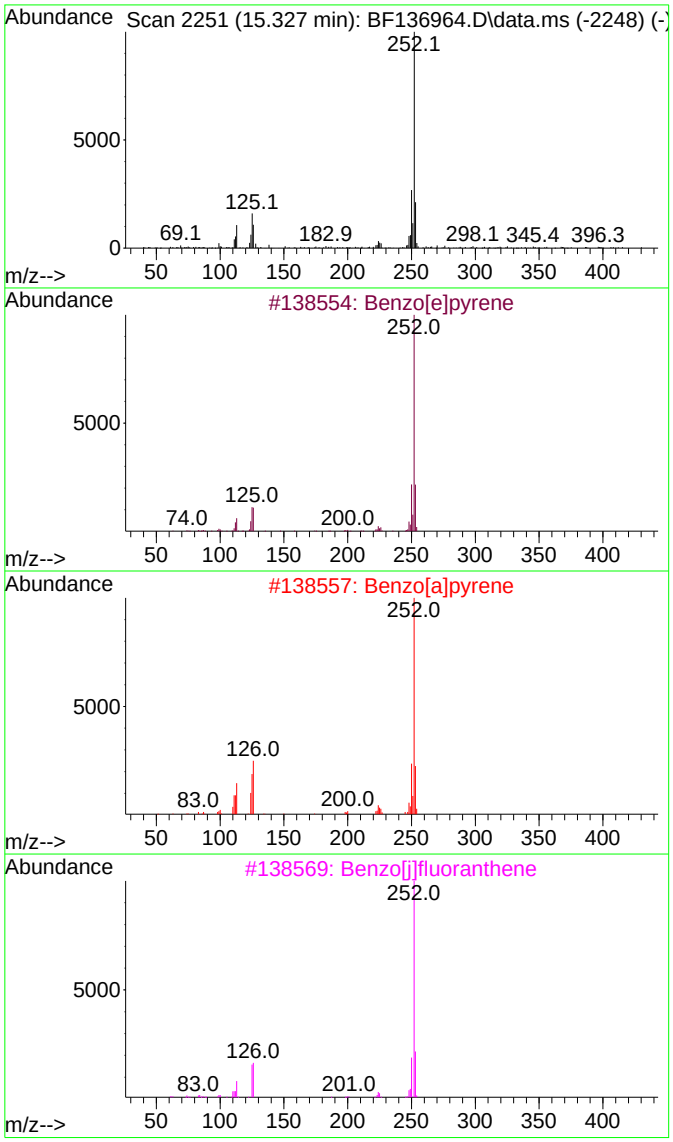
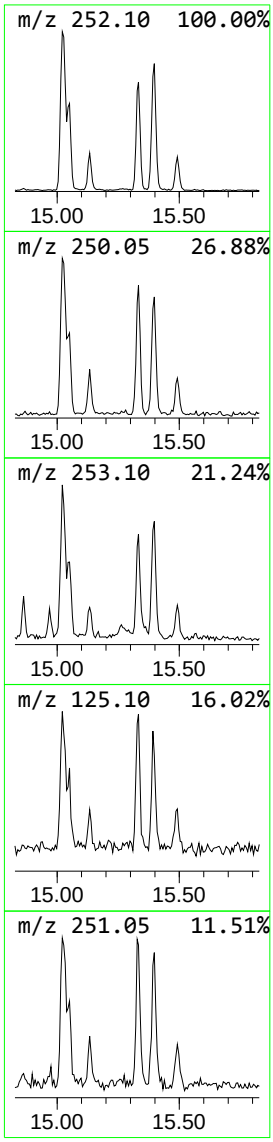
Peak Number 12 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	15.99 ng	157242	Perylene-d12	15.457

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	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136964.D
Acq On : 05 Jan 2024 03:34
Operator : CG\JU
Sample : 06045-01
Misc :
ALS Vial : 22 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-...	4.999	7.0	ng	84799	1	6.781	242576	20.0
Anthracene, 9-m...	11.816	2.8	ng	43813	4	11.310	313887	20.0
n-Hexadecanoic ...	11.845	10.4	ng	162561	4	11.310	313887	20.0
4H-Cyclopenta[d...	11.928	4.6	ng	71879	4	11.310	313887	20.0
Phenanthrene, 2...	12.369	2.0	ng	32139	4	11.310	313887	20.0
Cyclopenta(def)...	12.457	2.3	ng	36119	4	11.310	313887	20.0
Pyrene, 1-methyl-	13.092	3.3	ng	107814	5	13.969	647900	20.0
Pyrene, 4-methyl-	13.198	2.0	ng	65702	5	13.969	647900	20.0
Triphenylphosph...	14.063	3.0	ng	96243	5	13.969	647900	20.0
Benzo[e]pyrene	15.327	16.0	ng	157242	6	15.457	196658	20.0