LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-323-6-8

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: BF136979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	495	498	506	rBV	28917	33292	3.02%	0.306%
2	5.428	564	568	584	rBV	1105245	1002244	90.99%	9.208%
3	6.434	735	739	755	rBV	1092400	983641	89.31%	9.037%
4	6.781	795	798	802	rBV	398410	314462	28.55%	2.889%
5	7.345	890	894	897	rBV	747542	619423	56.24%	5.691%
6	8.057	1012	1015	1021	rBV	452598	382055	34.69%	3.510%
7	8.469	1082	1085	1095	rBV3	9029	13970	1.27%	0.128%
8	9.133	1194	1198	1202	rBV	1294345	1101430	100.00%	10.119%
9	9.475	1252	1256	1258	rBV	18878	17439	1.58%	0.160%
10	9.674	1287	1290	1294	rBV	29182	25249	2.29%	0.232%
11	9.816	1310	1314	1318	rBV	457756	367017	33.32%	3.372%
12	9.851	1318	1320	1324	rVB2	15055	13620	1.24%	0.125%
13	10.022	1344	1349	1353	rBV2	17685	18154	1.65%	0.167%
14	10.369	1404	1408	1413	rVB2	31421	32883	2.99%	0.302%
15	10.610	1445	1449	1460	rVB	615035	538682	48.91%	4.949%
16	10.733	1465	1470	1475	rVB5	9873	17356	1.58%	0.159%
17	10.916	1495	1501	1504	rBV4	14325	19003	1.73%	0.175%
18	11.204	1547	1550	1555	rVB	22150	19737	1.79%	0.181%
19	11.310	1564	1568	1570	rBV	427479	360860	32.76%	3.315%
20	11.333	1570	1572	1575	rVV	305458	229618	20.85%	2.110%
21	11.386	1577	1581	1584	rVB	55599	49050	4.45%	0.451%
22	11.551	1606	1609	1613	rBV2	10251	12412	1.13%	0.114%
23	11.639	1620	1624	1630	rVB2	15420	20293	1.84%	0.186%
24	11.727	1633	1639	1642	rVB3	9293	12705	1.15%	0.117%
25	11.816	1650	1654	1656	rBV	57622	54773	4.97%	0.503%
26	11.839	1656	1658	1664	rVV	152759	159514	14.48%	1.466%
27	11.892	1664	1667	1669	rVV	25951	28589	2.60%	0.263%
28	11.927	1669	1673	1675	rVV2	79020	88854	8.07%	0.816%
29	11.951	1675	1677	1683	rVB	44155	36486	3.31%	0.335%
30	12.092	1697	1701	1702	rBV4	16402	15696	1.43%	0.144%
31	12.110	1702	1704	1707	rVV	33927	30885	2.80%	0.284%
32	12.145	1707	1710	1712	rVB	17982	17087	1.55%	0.157%
33	12.292	1732	1735	1737	rBV	17763	13789	1.25%	0.127%
34	12.368	1742	1748	1750	rBV	44367	47686	4.33%	0.438%
35	12.404	1750	1754	1756	rVV3	29719	34395	3.12%	0.316%
36	12.457	1760	1763	1767	rBV4	23423	29422	2.67%	0.270%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MR-323-6-8

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	12.527	1772	1775	1779	rBV	339734	297017	26.97%	2.729%
38	12.627	1789	1792	1796	rBV2	26855	28945	2.63%	0.266%
39	12.680	1798	1801	1804	rVB2	17028	18113	1.64%	0.166%
40	12.757	1809	1814	1820	rVV	297238	335222	30.44%	3.080%
41	12.815	1820	1824	1828	rVB3	20814	27988	2.54%	0.257%
42	12.904	1835	1839	1842	rBV	1224874	1019237	92.54%	9.364%
43	12.980	1847	1852	1856	rBV3	30407	50995	4.63%	0.469%
44	13.092	1868	1871	1874	rVB2	52452	54151	4.92%	0.498%
45	13.133	1875	1878	1880	rBV3	12928	14154	1.29%	0.130%
46	13.157	1880	1882	1885	rVV	41784	35266	3.20%	0.324%
47	13.198	1885	1889	1896	rVB2	47811	61525	5.59%	0.565%
48	13.286	1901	1904	1907	rVB	32012	27222	2.47%	0.250%
49	13.321	1907	1910	1913	rBV	32473	35226	3.20%	0.324%
50	13.445	1928	1931	1933	rBV2	16220	12607	1.14%	0.116%
51	13.480	1933	1937	1939	rBV4	18967	22792	2.07%	0.209%
52	13.580	1951	1954	1955	rBV3	13338	15386	1.40%	0.141%
53	13.604	1956	1958	1962	rVB	28988	29790	2.70%	0.274%
54	13.715	1974	1977	1980	rBV	32946	29318	2.66%	0.269%
55	13.739	1980	1981	1984	rVB	26459	16917	1.54%	0.155%
56	13.815	1991	1994	1997	rVB2	34214	35104	3.19%	0.323%
57	13.868	1997	2003	2009	rBV6	34966	107857	9.79%	0.991%
58	13.968	2015	2020	2022	rBV2	478368	557618	50.63%	5.123%
59	13.992	2022	2024	2028	rVB	163112	133443	12.12%	1.226%
60	14.062	2033	2036	2040	rVB3	35578	48556	4.41%	0.446%
61	14.121	2043	2046	2052	rBV5	25204	38313	3.48%	0.352%
62	14.321	2077	2080	2081	rBV	16375	16313	1.48%	0.150%
63	14.357	2084	2086	2090	rVV	46974	43022	3.91%	0.395%
64	14.392	2090	2092	2096	rVB	25837	21496	1.95%	0.197%
65	14.433	2097	2099	2101	rVV3	23549	25927	2.35%	0.238%
66	14.480	2105	2107	2109	rVV	24554	19673	1.79%	0.181%
67	15.021	2194	2199	2202	rBV	121238	194052	17.62%	1.783%
68	15.127	2215	2217	2222	rBV	21182	20615	1.87%	0.189%
69	15.327	2247	2251	2254	rBV	66229	81697	7.42%	0.751%
70	15.392	2258	2262	2268	rVB	94212	122687	11.14%	1.127%
71	15.456	2268	2273	2277	rBV	306165	402483	36.54%	3.698%
72	16.968	2526	2530	2537	rVB3	35317	65949	5.99%	0.606%
73	17.433	2605	2609	2618	rVB3	26315	55787	5.06%	0.513%

Sum of corrected areas: 10884234

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Acq On : 05 Jan 2024 16:55
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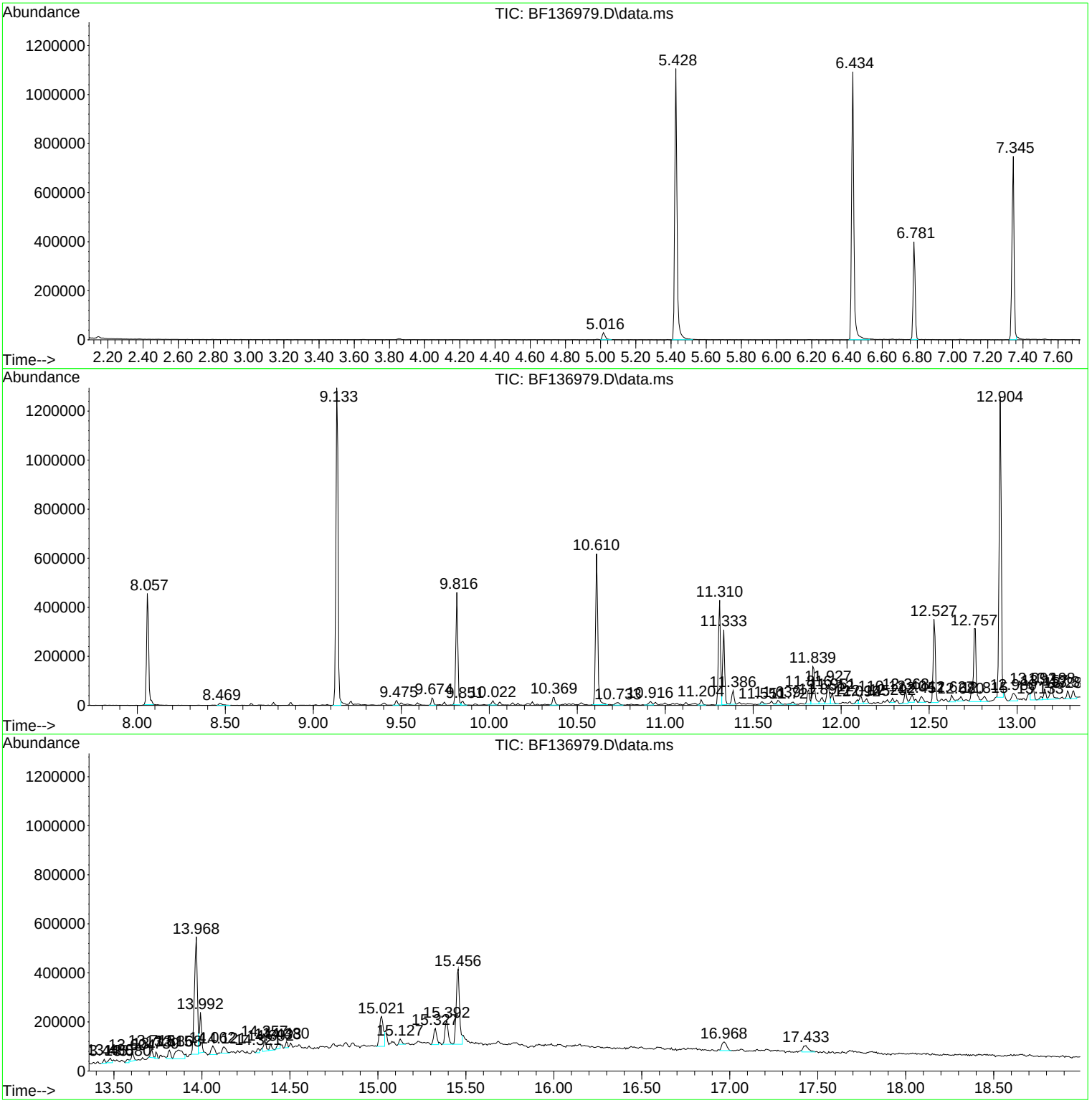
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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\BF010524\
Data File : BF136979.D
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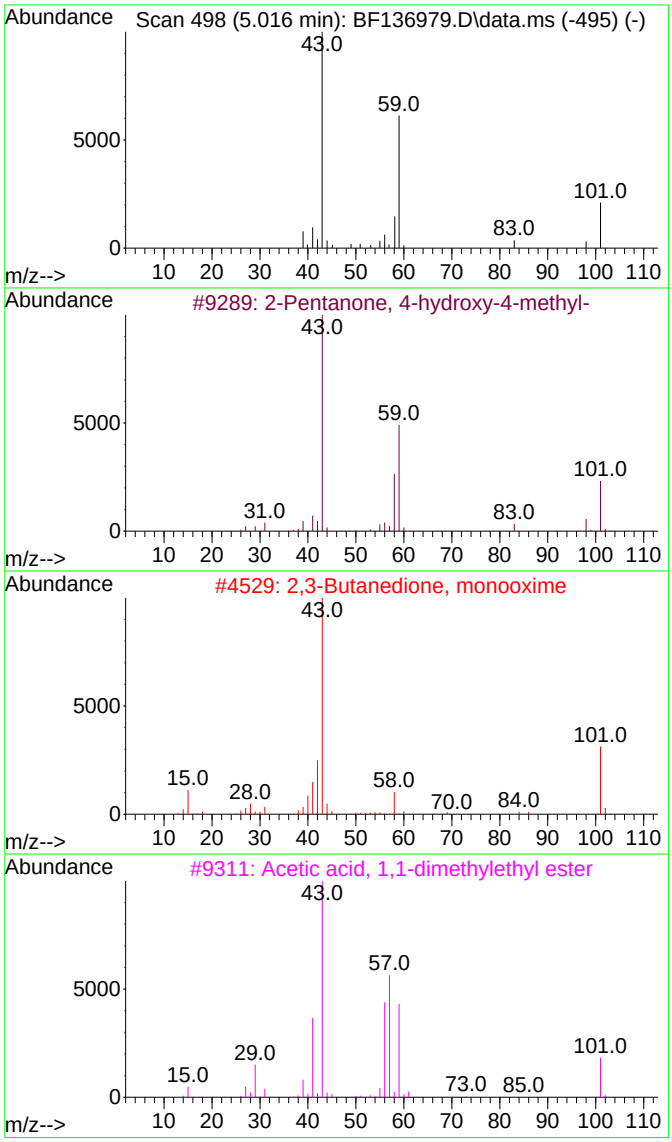
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

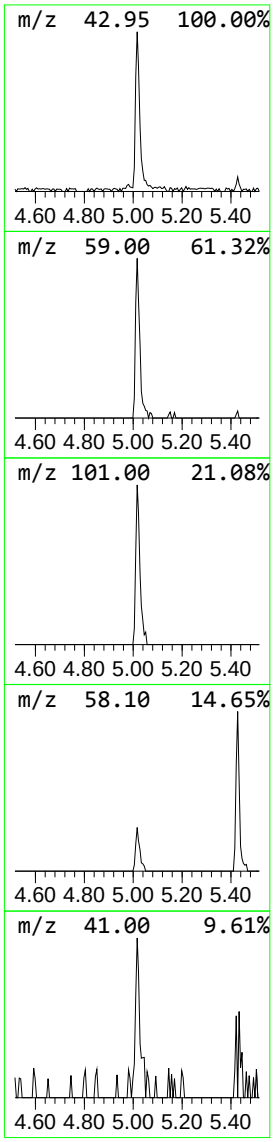
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.12 ng	33292	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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

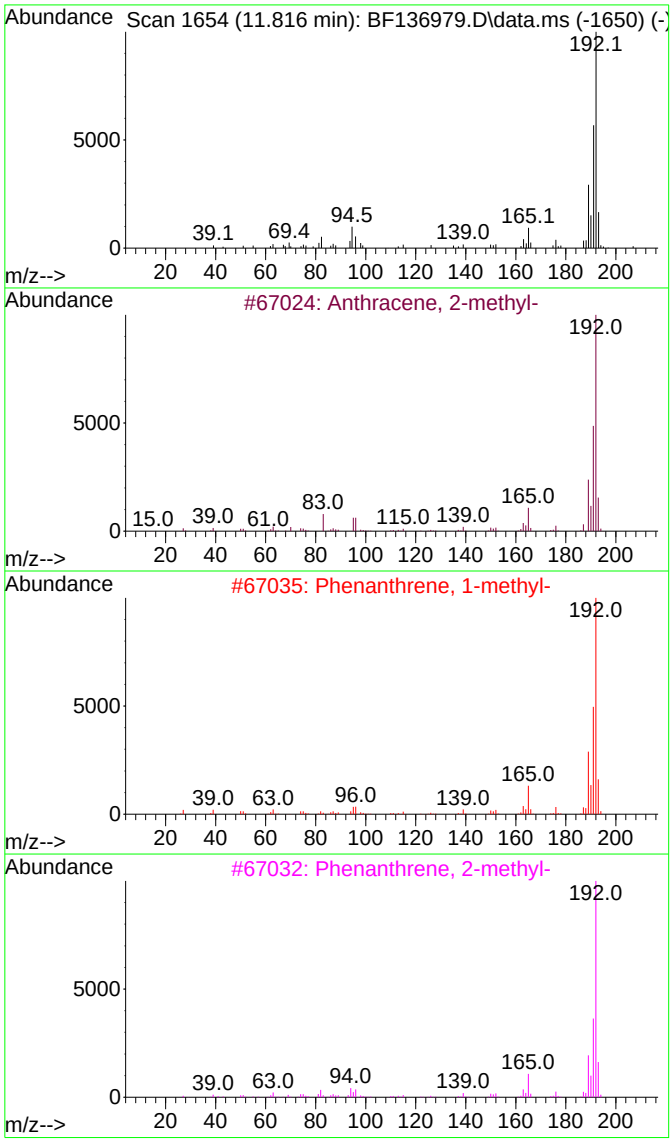
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

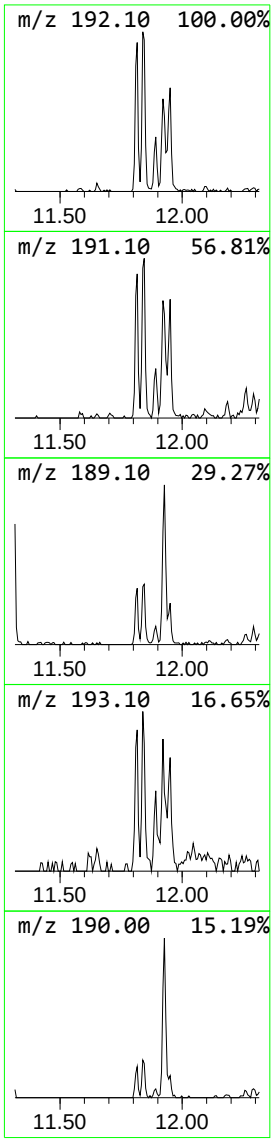
****

Peak Number 2 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	3.04 ng	54773	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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

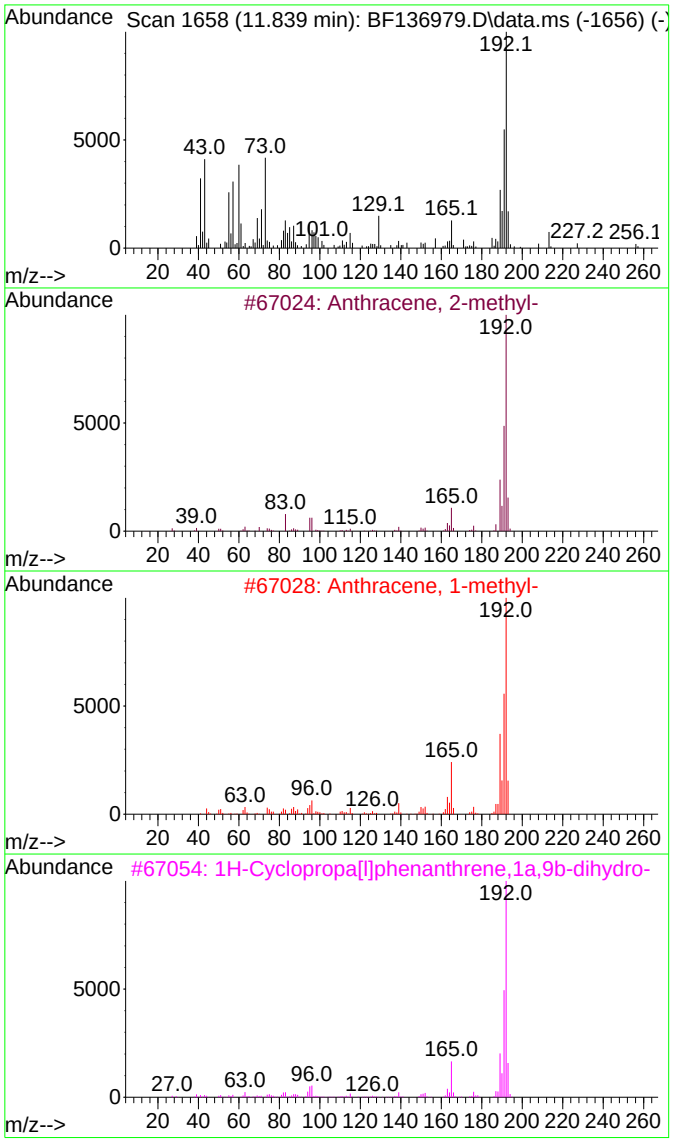
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

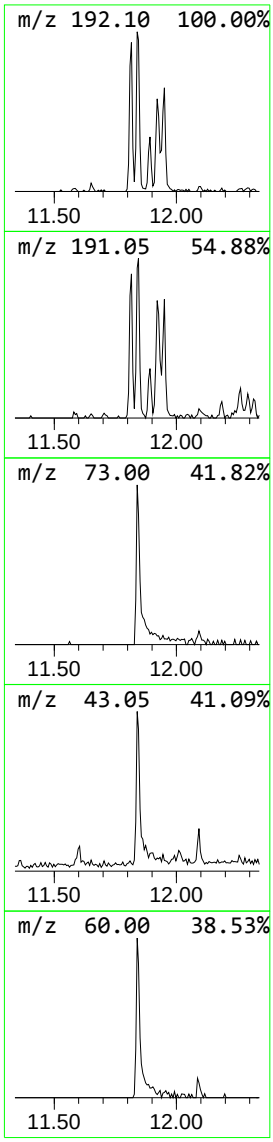
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	8.84 ng	159514	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	92
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

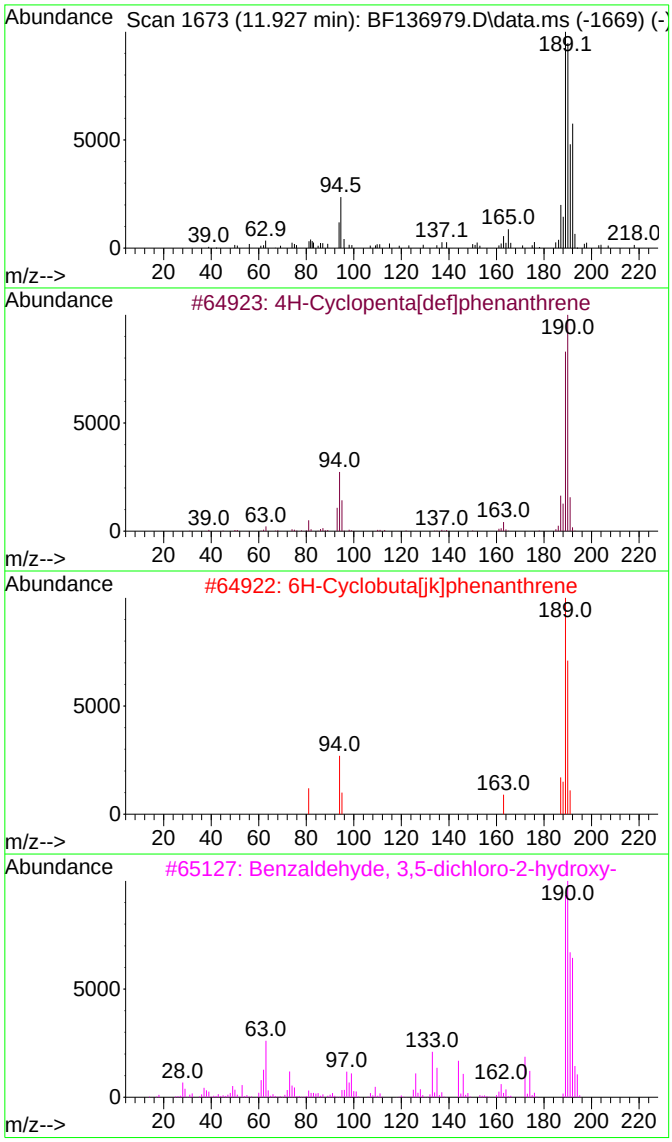
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

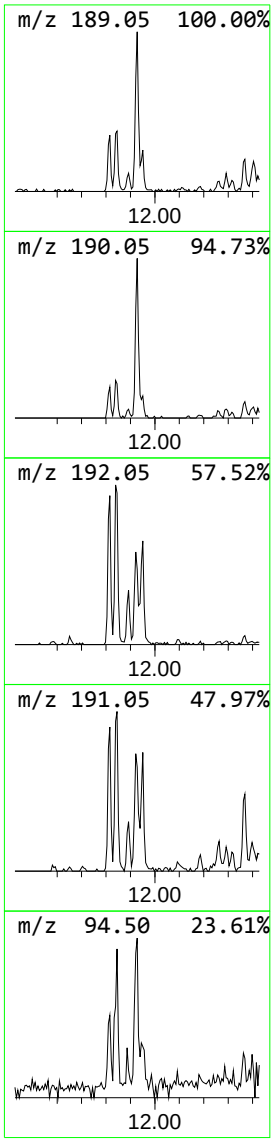
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	4.92 ng	88854	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	47
5	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38





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Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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

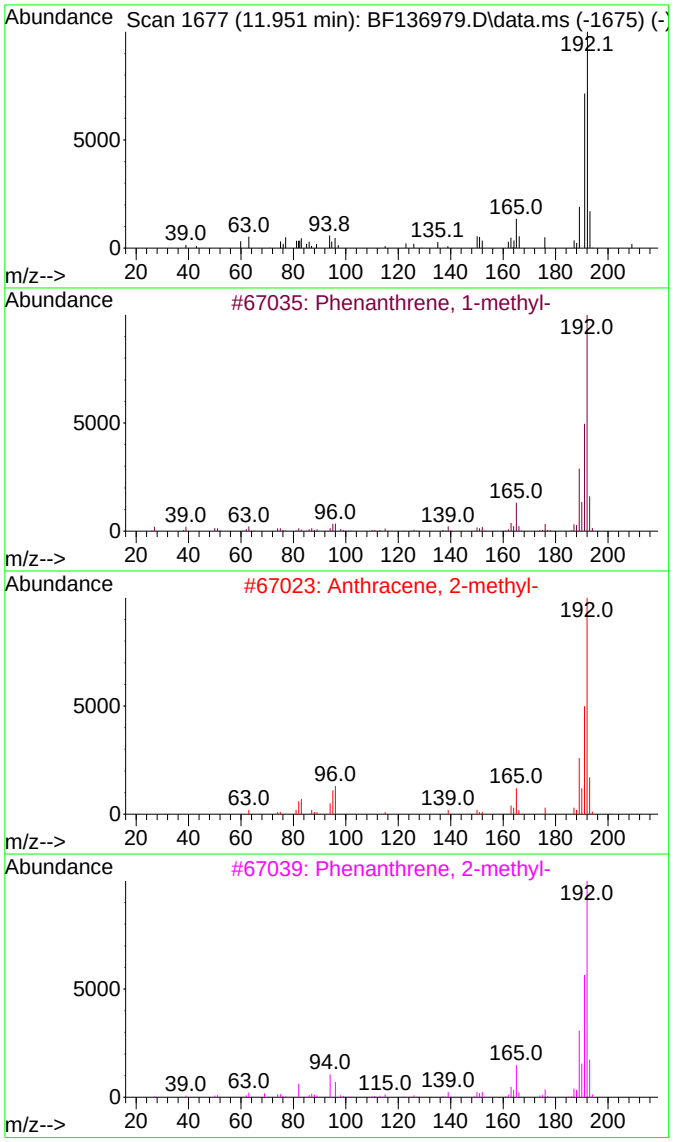
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

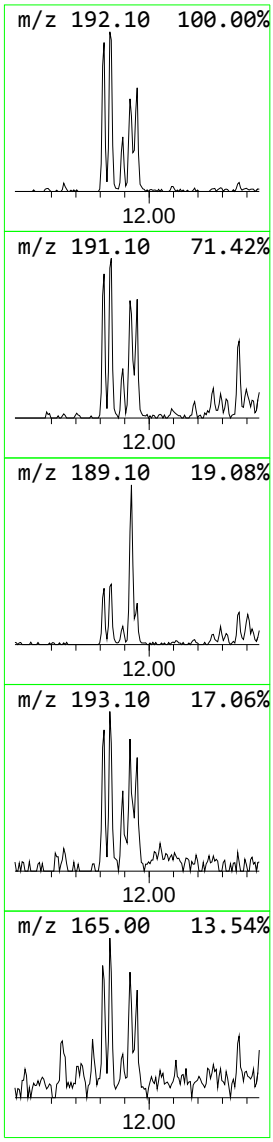
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.02 ng	36486	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	87
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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

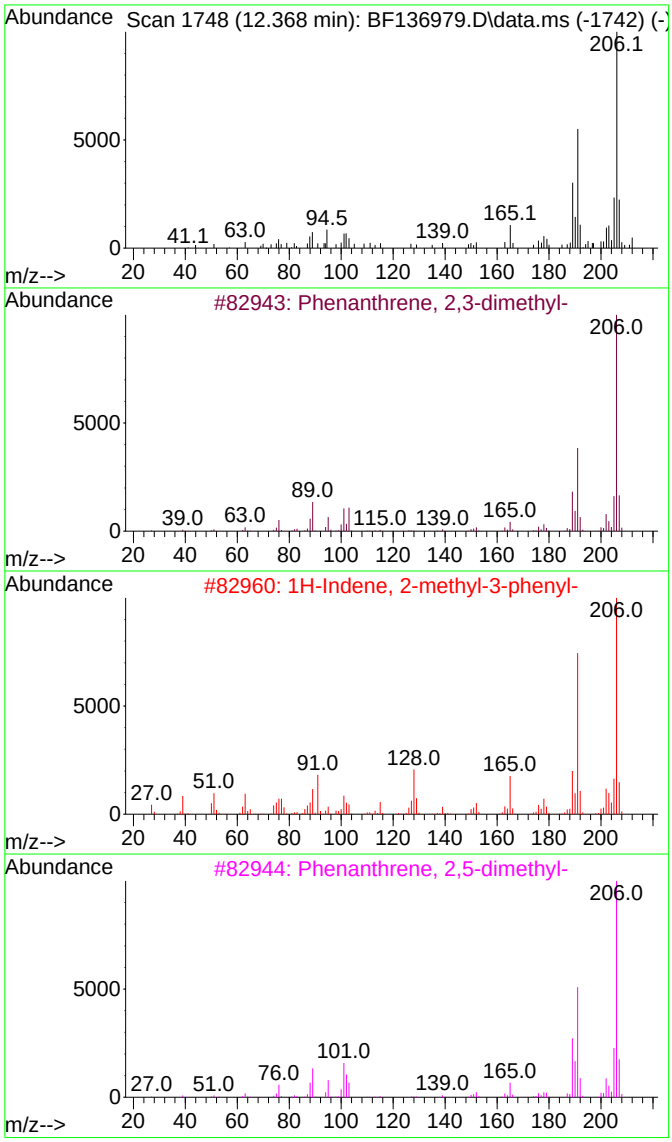
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

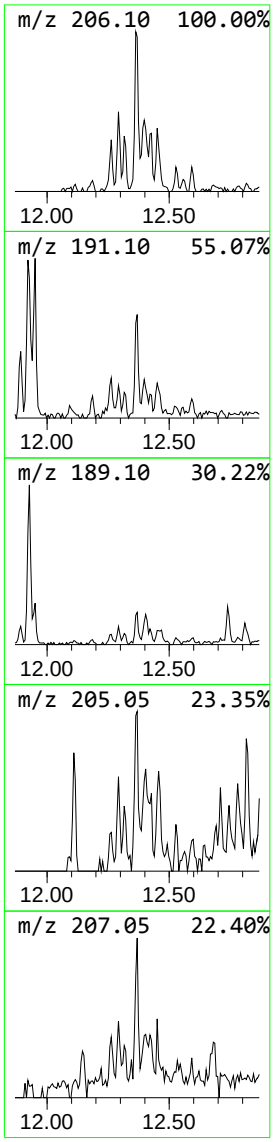
****

Peak Number 6 Phenanthrene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.368	2.64 ng	47686	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
2	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	91
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
4	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
5	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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

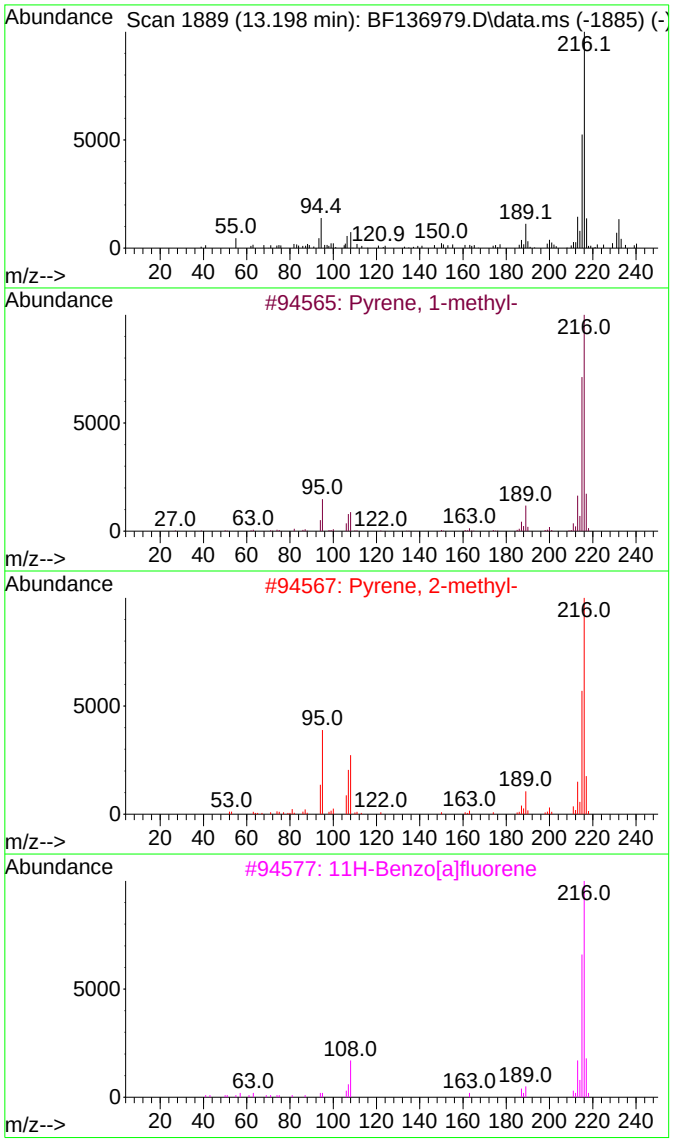
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

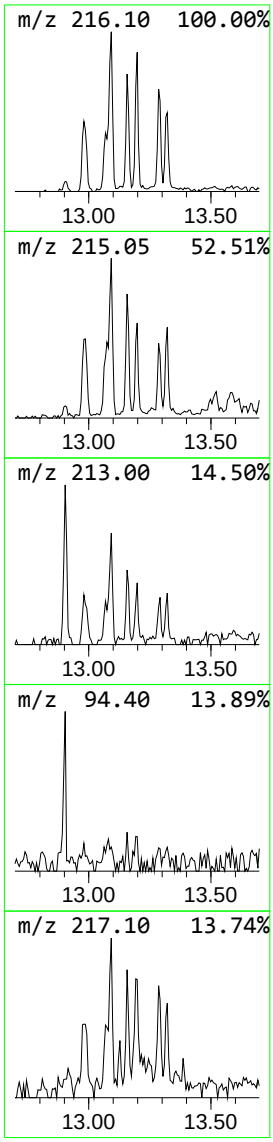
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.198	2.21 ng	61525	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	68





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Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MR-323-6-8

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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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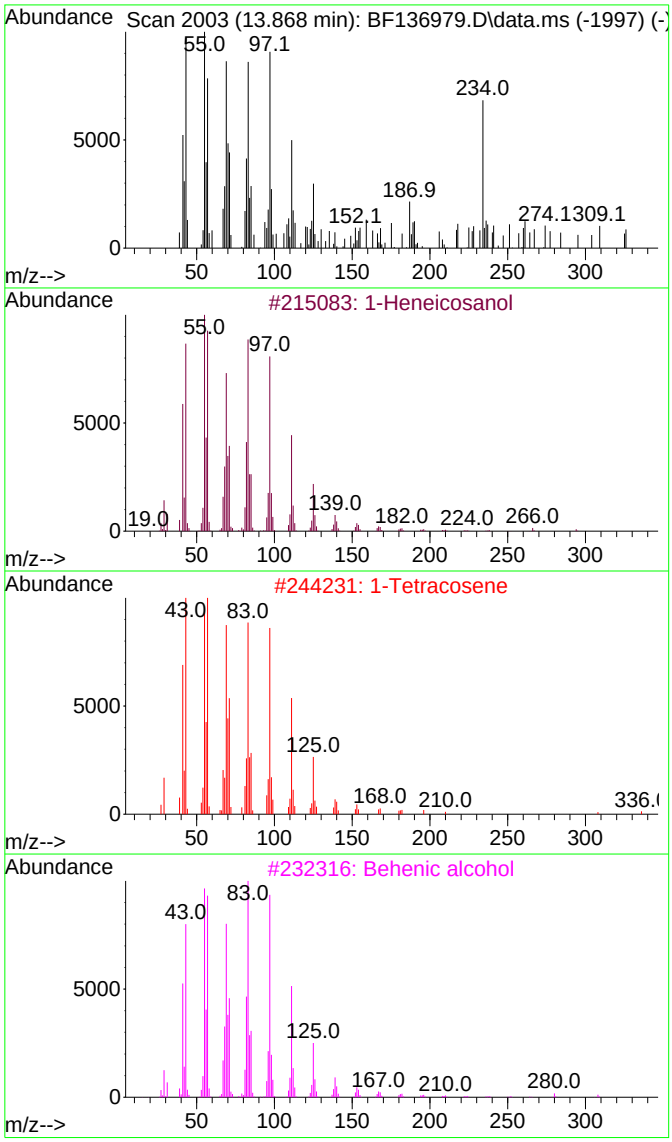
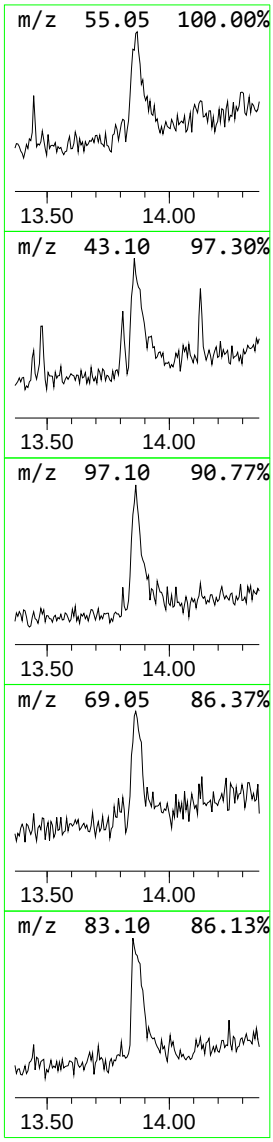
Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	3.87 ng	107857	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	76
2	1-Tetracosene	336	C24H48	010192-32-2	76
3	Behenic alcohol	326	C22H46O	000661-19-8	76
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	68
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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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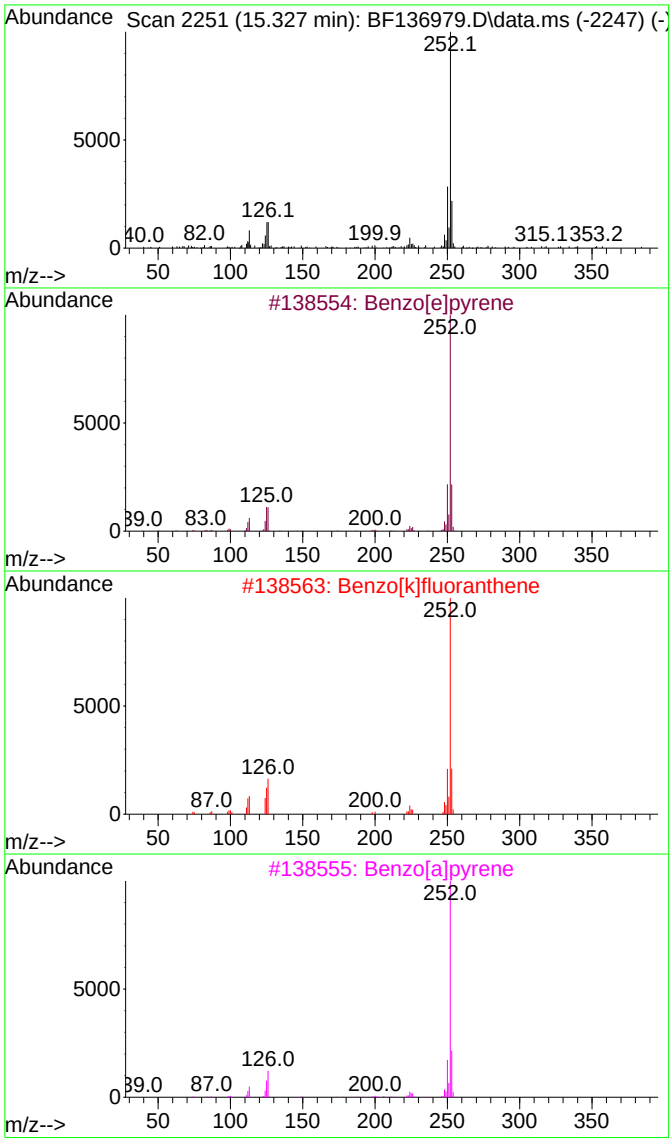
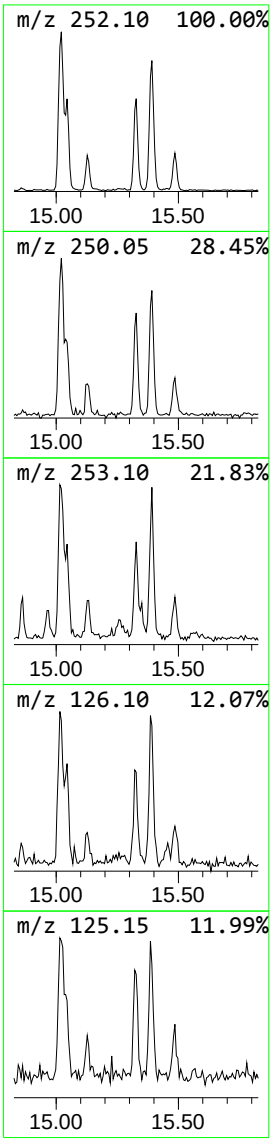
Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	4.06 ng	81697	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[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136979.D
Acq On : 05 Jan 2024 16:55
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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-...	5.016	2.1	ng	33292	1	6.781	314462	20.0
Anthracene, 2-m...	11.816	3.0	ng	54773	4	11.310	360860	20.0
Anthracene, 1-m...	11.839	8.8	ng	159514	4	11.310	360860	20.0
4H-Cyclopenta[d...	11.927	4.9	ng	88854	4	11.310	360860	20.0
Phenanthrene, 1...	11.951	2.0	ng	36486	4	11.310	360860	20.0
Phenanthrene, 2...	12.368	2.6	ng	47686	4	11.310	360860	20.0
Pyrene, 1-methyl-	13.198	2.2	ng	61525	5	13.968	557618	20.0
1-Heneicosanol	13.868	3.9	ng	107857	5	13.968	557618	20.0
Benzo[e]pyrene	15.327	4.1	ng	81697	6	15.457	402483	20.0