LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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: BF136957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	493	496	502	rBV	25742	28665	2.93%	0.305%
2	5.422	564	567	584	rBV	943222	859371	87.76%	9.134%
3	6.428	735	738	754	rBV	849847	869688	88.81%	9.244%
4	6.781	795	798	802	rBV	360147	264963	27.06%	2.816%
5	7.345	890	894	897	rBV	602040	537810	54.92%	5.716%
6	8.057	1012	1015	1018	rBV	416082	322087	32.89%	3.423%
7	8.469	1081	1085	1096	rVB2	7914	14130	1.44%	0.150%
8	9.134	1194	1198	1201	rBV	1274651	979245	100.00%	10.408%
9	9.475	1253	1256	1258	rBV	17132	16549	1.69%	0.176%
10	9.675	1287	1290	1293	rBV	24707	19827	2.02%	0.211%
11	9.816	1310	1314	1317	rBV	409129	342974	35.02%	3.645%
12	9.845	1317	1319	1323	rVB2	14208	12865	1.31%	0.137%
13	10.022	1344	1349	1353	rBV2	17783	18942	1.93%	0.201%
14	10.363	1404	1407	1413	rVB	35305	33536	3.42%	0.356%
15	10.610	1445	1449	1461	rVV	583282	512695	52.36%	5.449%
16	10.728	1465	1469	1475	rVB4	11023	15785	1.61%	0.168%
17	10.916	1496	1501	1504	rBV3	14626	16226	1.66%	0.172%
18	11.204	1547	1550	1554	rVB	19949	17457	1.78%	0.186%
19	11.310	1564	1568	1570	rBV	386123	353661	36.12%	3.759%
20	11.333	1570	1572	1575	rVV	269552	206266	21.06%	2.192%
21	11.386	1575	1581	1584	rVB	46900	46229	4.72%	0.491%
22	11.551	1604	1609	1613	rBV3	11377	16786	1.71%	0.178%
23	11.639	1622	1624	1629	rVB3	16229	17487	1.79%	0.186%
24	11.810	1650	1653	1656	rBV	54189	48953	5.00%	0.520%
25	11.839	1656	1658	1663	rVV	157798	149163	15.23%	1.585%
26	11.886	1664	1666	1669	rVV	24874	27765	2.84%	0.295%
27	11.922	1669	1672	1675	rVV	72886	81912	8.36%	0.871%
28	11.945	1675	1676	1682	rVB	36188	30241	3.09%	0.321%
29	12.092	1697	1701	1702	rBV2	16658	16573	1.69%	0.176%
30	12.110	1702	1704	1707	rVV	32693	29444	3.01%	0.313%
31	12.139	1707	1709	1713	rVB3	16573	15393	1.57%	0.164%
32	12.292	1732	1735	1737	rVB	15574	12944	1.32%	0.138%
33	12.363	1744	1747	1750	rBV	38718	42148	4.30%	0.448%
34	12.398	1750	1753	1756	rVV3	30081	37024	3.78%	0.394%
35	12.457	1759	1763	1766	rBV3	20746	26422	2.70%	0.281%
36	12.527	1771	1775	1779	rBV	310338	255236	26.06%	2.713%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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	12.627	1789	1792	1797	rBV2	25130	37161	3.79%	0.395%
38	12.757	1809	1814	1820	rVV	268385	278704	28.46%	2.962%
39	12.816	1820	1824	1827	rVB3	17517	23918	2.44%	0.254%
40	12.904	1835	1839	1842	rBV	1063948	881098	89.98%	9.365%
41	12.975	1848	1851	1858	rBV5	26589	44212	4.51%	0.470%
42	13.063	1863	1866	1868	rVV3	20122	25973	2.65%	0.276%
43	13.086	1868	1870	1874	rVB	43011	42639	4.35%	0.453%
44	13.157	1880	1882	1884	rVB	30991	21914	2.24%	0.233%
45	13.192	1884	1888	1893	rBV2	40605	45604	4.66%	0.485%
46	13.286	1901	1904	1907	rVB	29244	23091	2.36%	0.245%
47	13.316	1907	1909	1912	rBV	29724	26032	2.66%	0.277%
48	13.380	1917	1920	1922	rBV2	14857	14032	1.43%	0.149%
49	13.445	1928	1931	1933	rBV	16940	16792	1.71%	0.178%
50	13.474	1933	1936	1939	rBV3	13886	19203	1.96%	0.204%
51	13.604	1956	1958	1962	rVB	20440	21752	2.22%	0.231%
52	13.710	1972	1976	1979	rBV2	29325	36012	3.68%	0.383%
53	13.739	1979	1981	1983	rVB	23515	16513	1.69%	0.176%
54	13.763	1983	1985	1991	rBV3	13731	21910	2.24%	0.233%
55	13.810	1991	1993	1997	rVB2	32256	32414	3.31%	0.345%
56	13.874	1997	2004	2005	rBV6	31566	64714	6.61%	0.688%
57	13.963	2013	2019	2022	rBV2	385163	508216	51.90%	5.402%
58	13.992	2022	2024	2029	rVB	145829	129423	13.22%	1.376%
59	14.063	2032	2036	2040	rVB3	23390	36049	3.68%	0.383%
60	14.122	2043	2046	2051	rBV6	25786	43129	4.40%	0.458%
61	14.357	2084	2086	2088	rVB	30758	24409	2.49%	0.259%
62	14.433	2097	2099	2104	rVB5	19773	24554	2.51%	0.261%
63	14.480	2105	2107	2109	rBV3	20318	15884	1.62%	0.169%
64	14.745	2150	2152	2154	rBV3	16670	12981	1.33%	0.138%
65	14.816	2162	2164	2167	rBV3	17754	15872	1.62%	0.169%
66	15.016	2194	2198	2201	rBV	102115	143350	14.64%	1.524%
67	15.321	2247	2250	2254	rBV	54623	54227	5.54%	0.576%
68	15.386	2257	2261	2267	rBV	85458	116168	11.86%	1.235%
69	15.451	2268	2272	2276	rBV	238351	294170	30.04%	3.127%

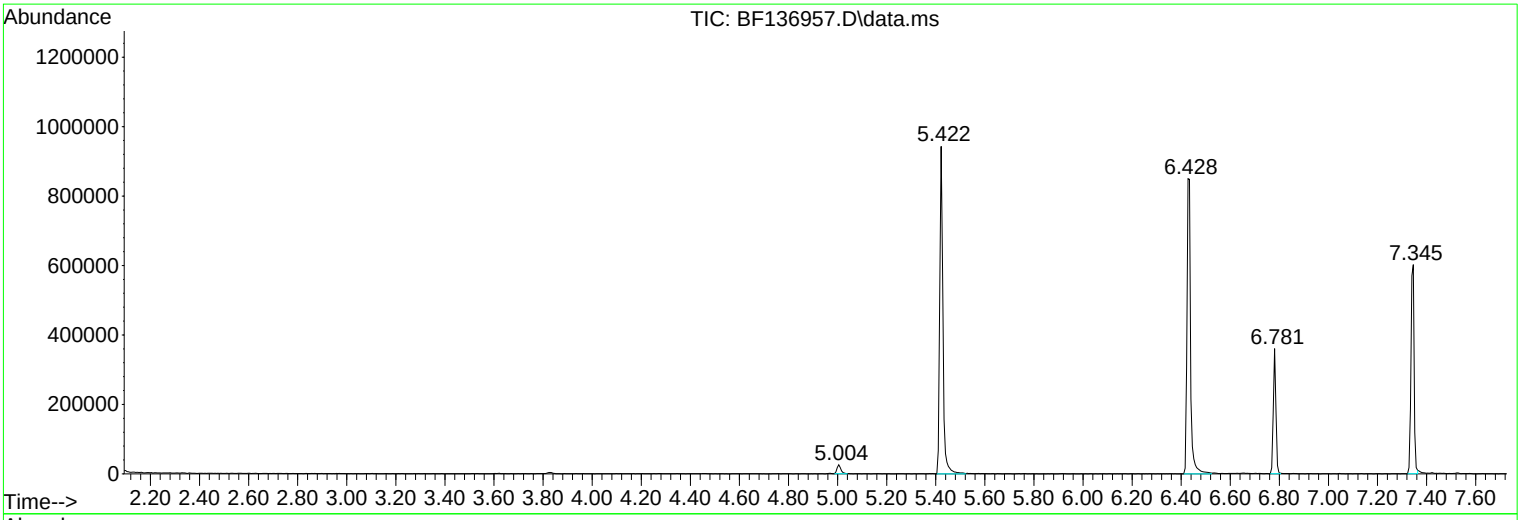
Sum of corrected areas: 9408582

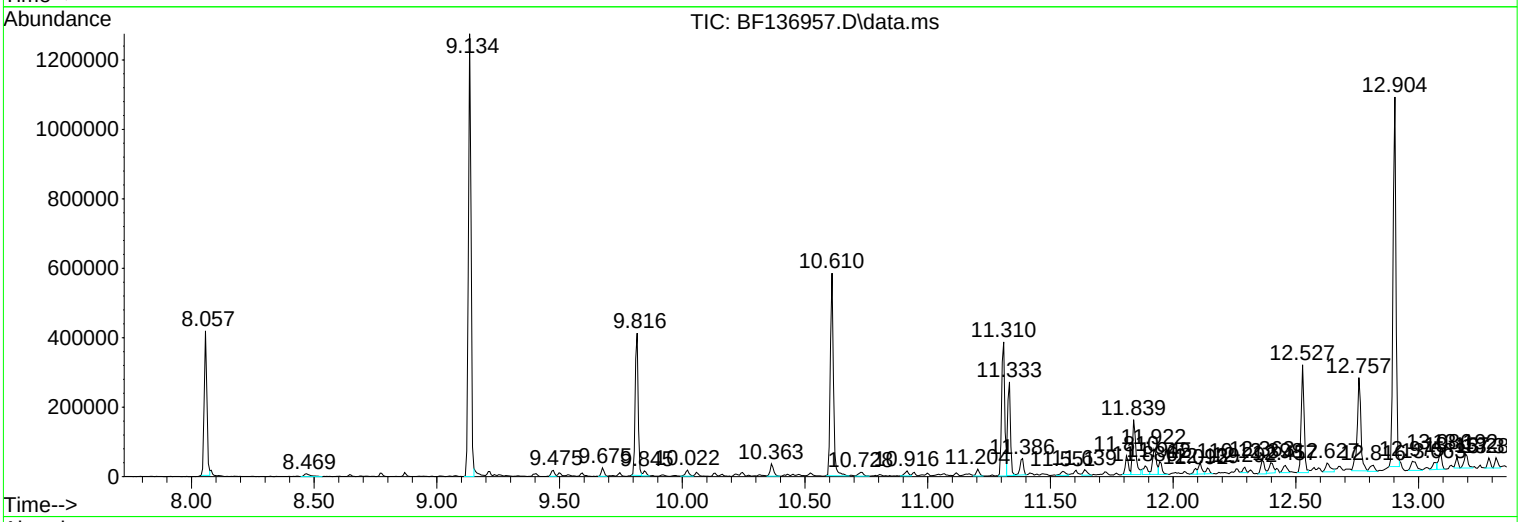
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

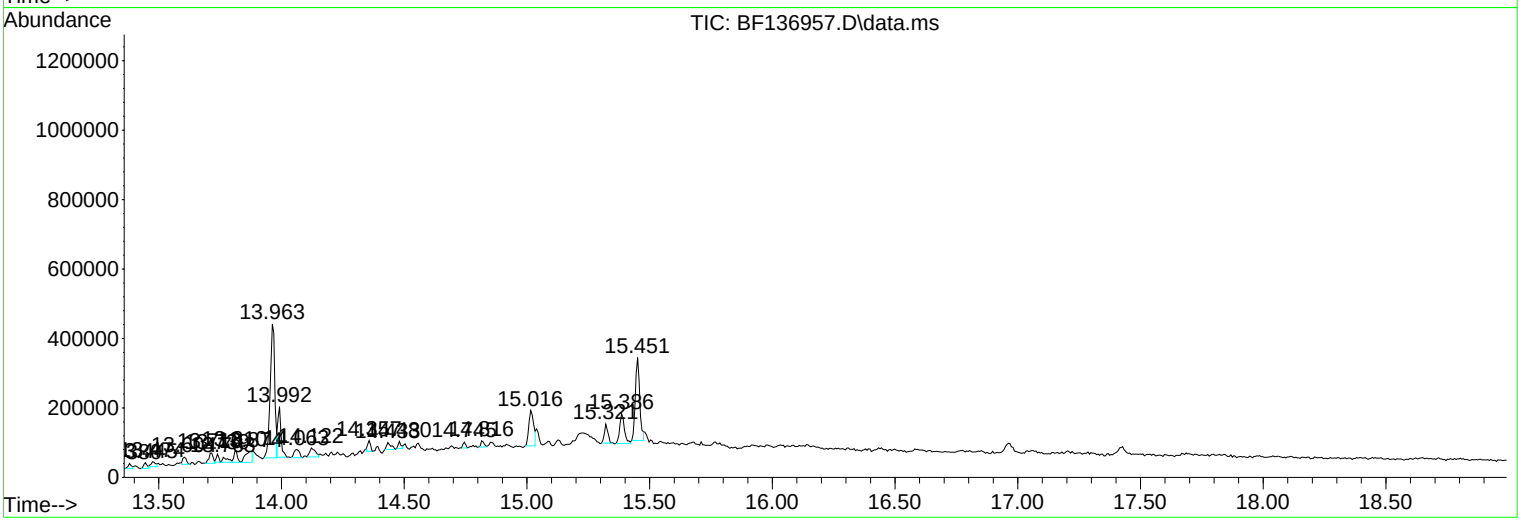
Instrument :
BNA_F
ClientSampleId :
MR-323-6-8

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\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

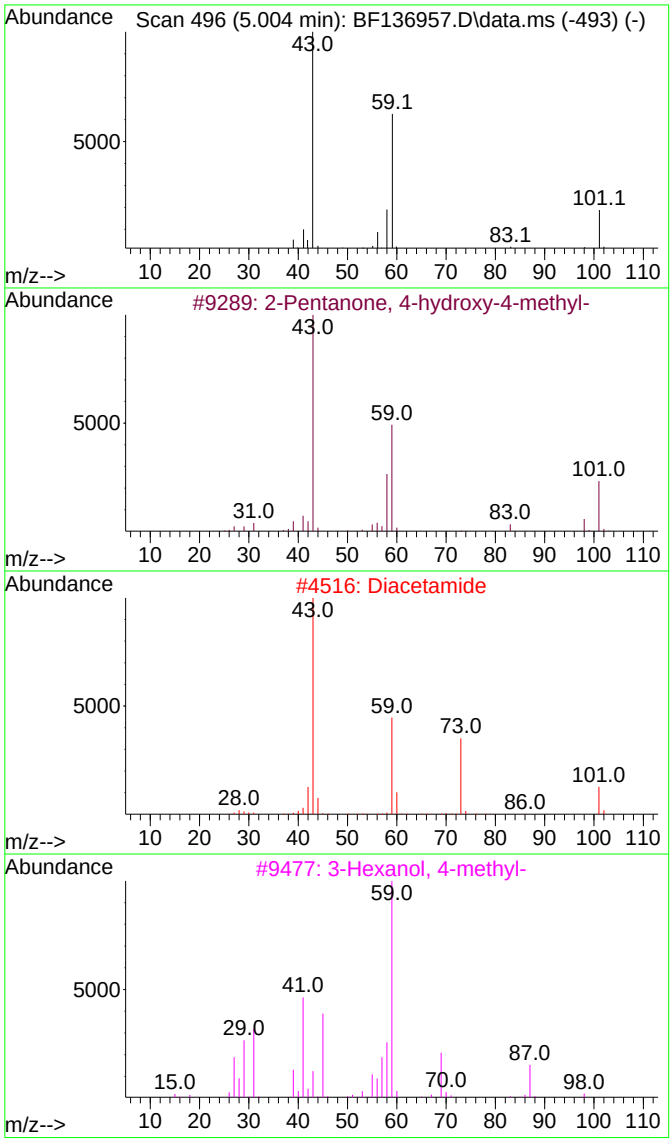
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

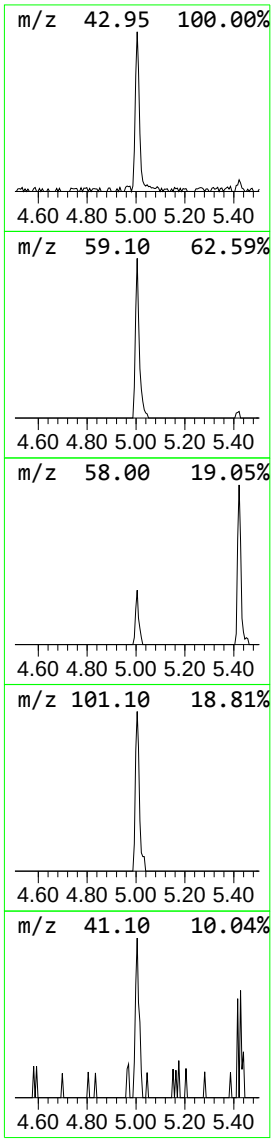
****

Peak Number 1 unknown5.004 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.16 ng	28665	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	45
2	Diacetamide	101	C4H7NO2	000625-77-4	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

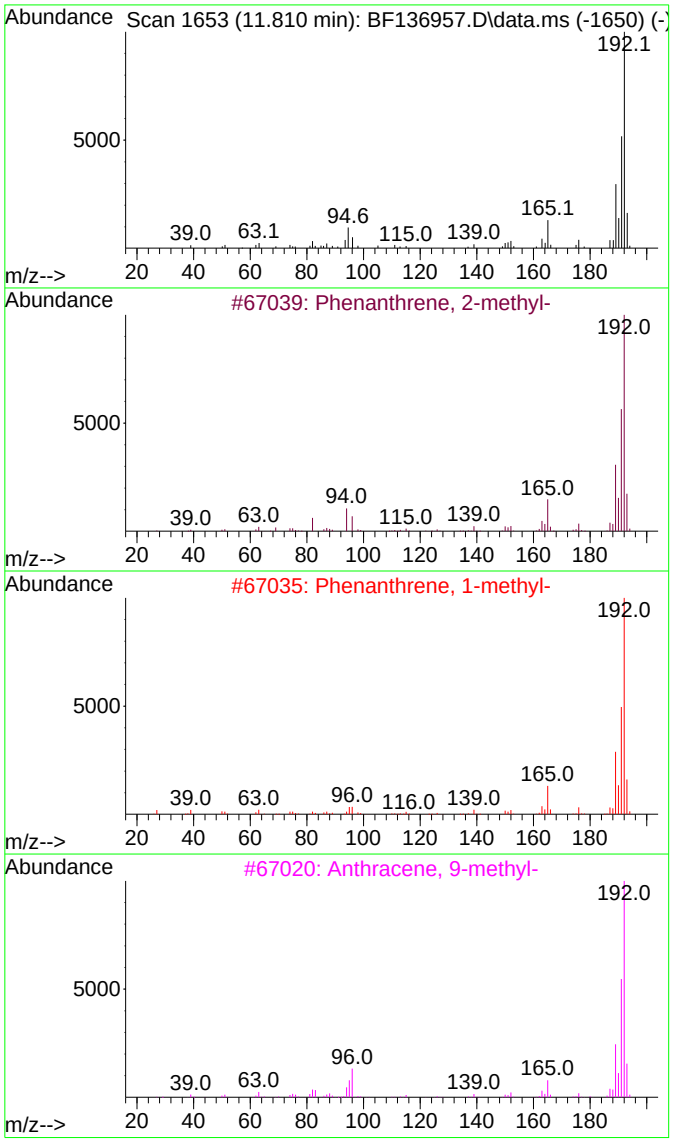
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

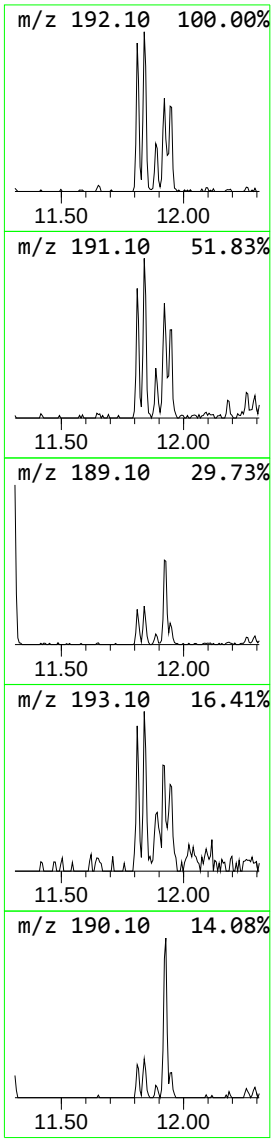
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.77 ng	48953	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

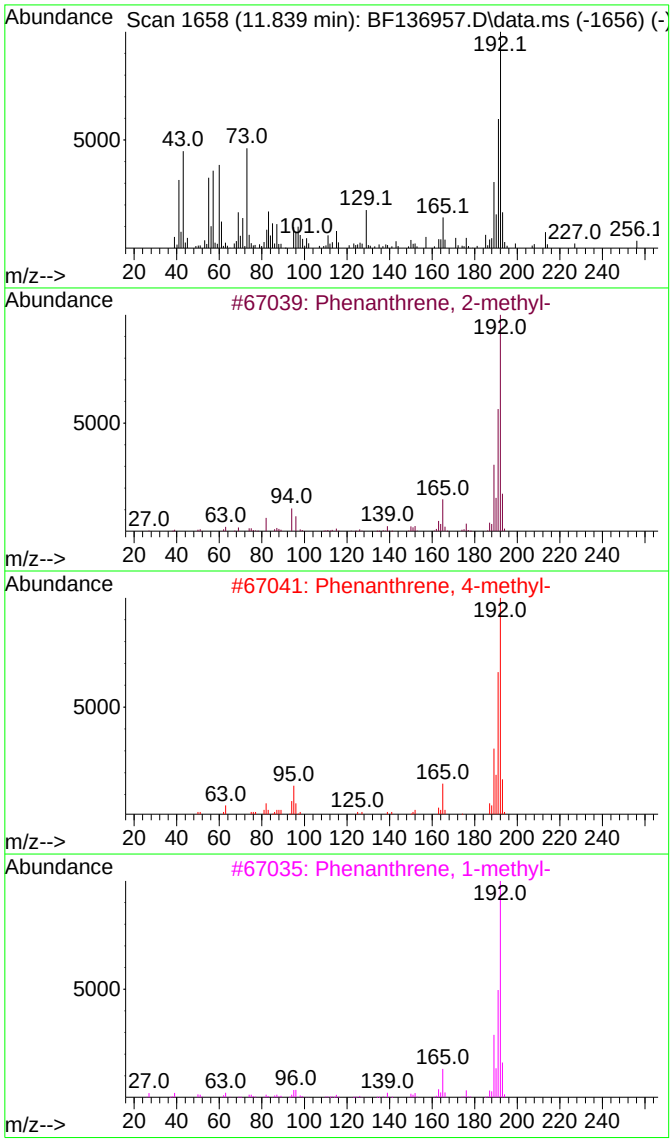
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

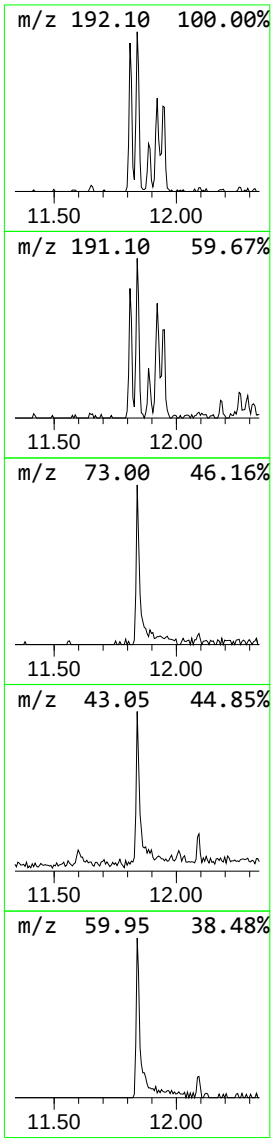
****

Peak Number 3 Phenanthrene, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	8.44 ng	149163	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

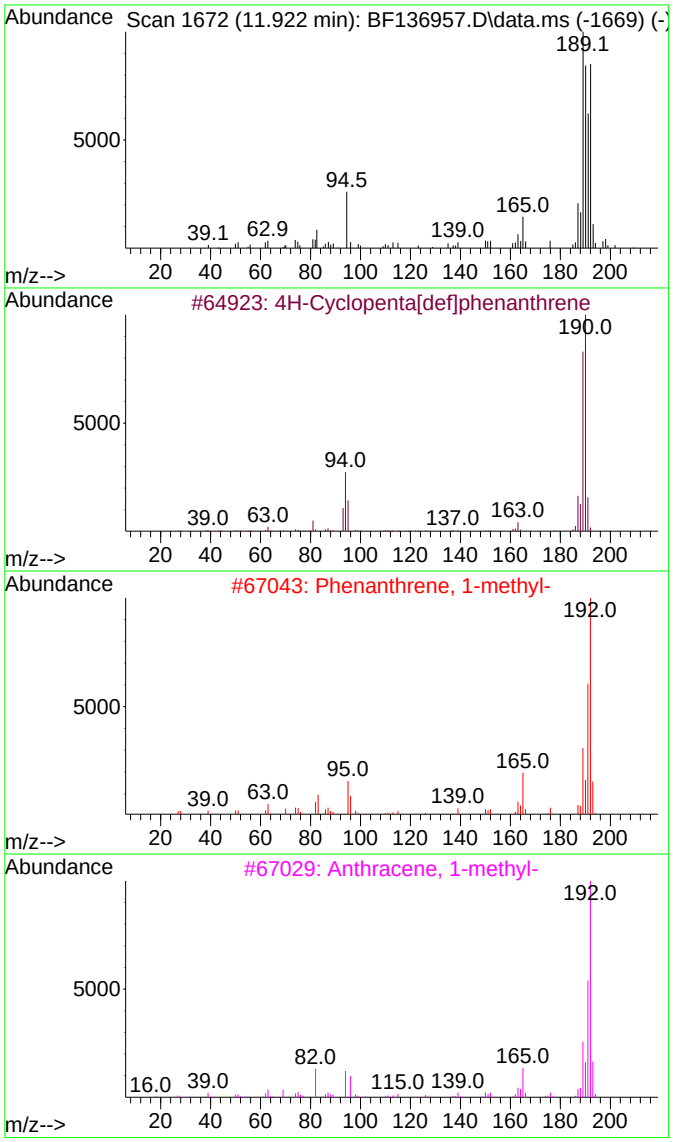
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

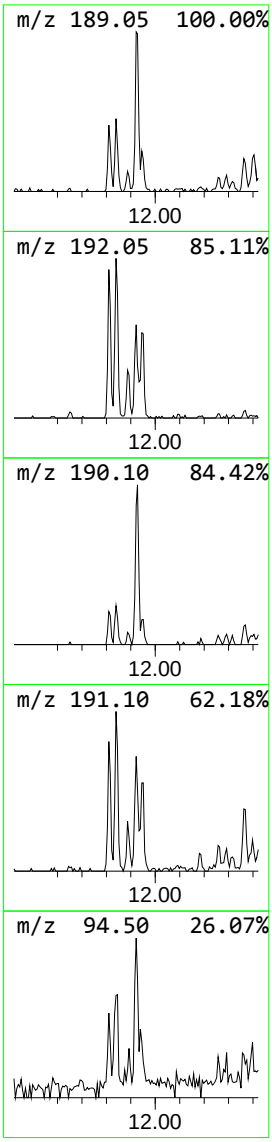
****

Peak Number 4 unknown11.922 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.63 ng	81912	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

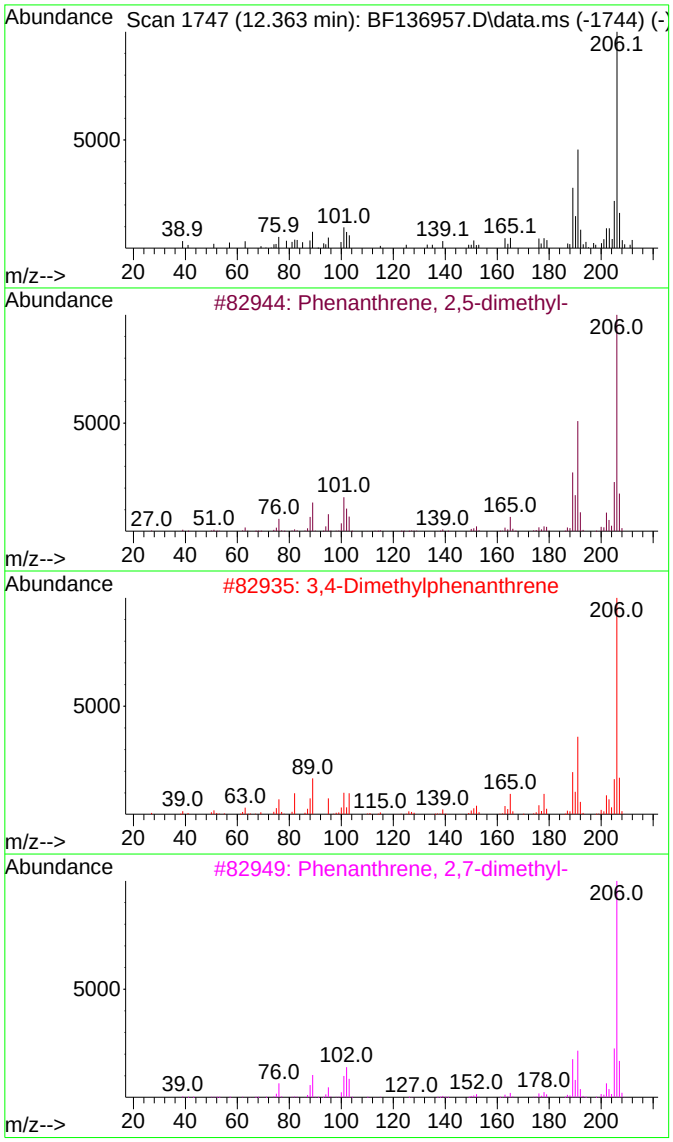
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

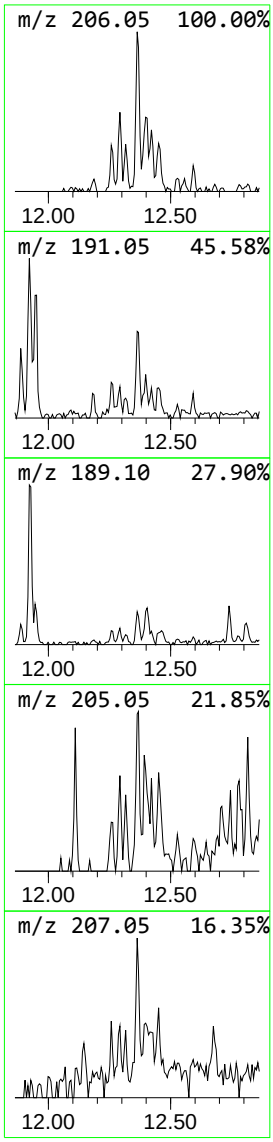
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	2.38 ng	42148	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	98
2	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	93
3	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	93
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

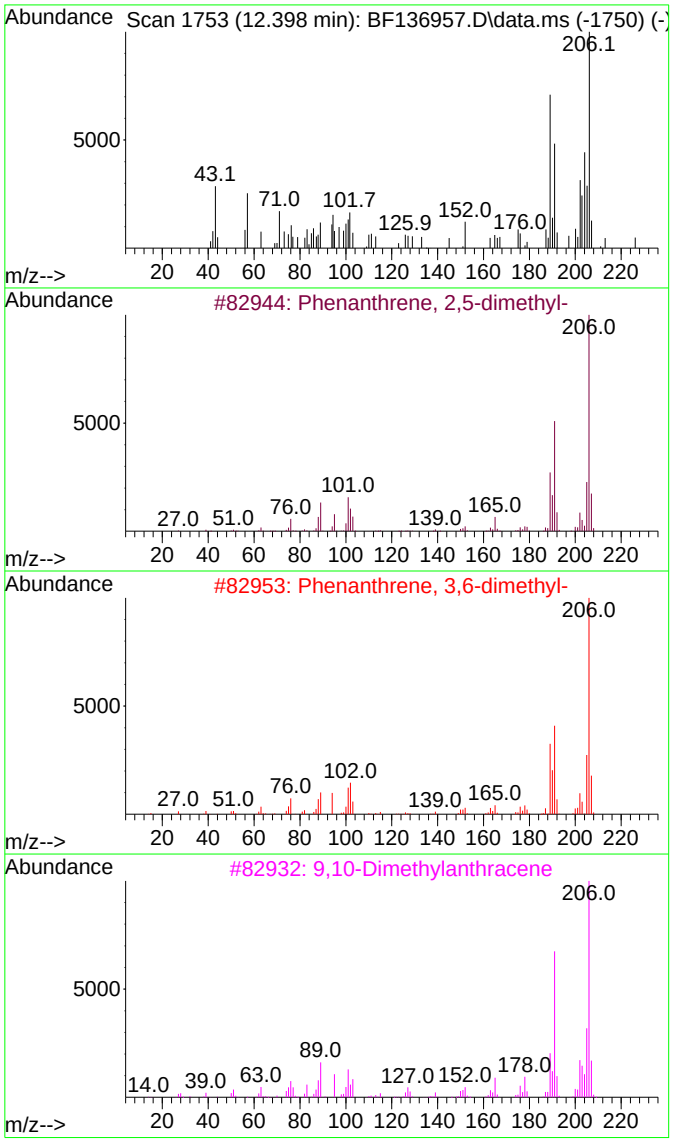
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

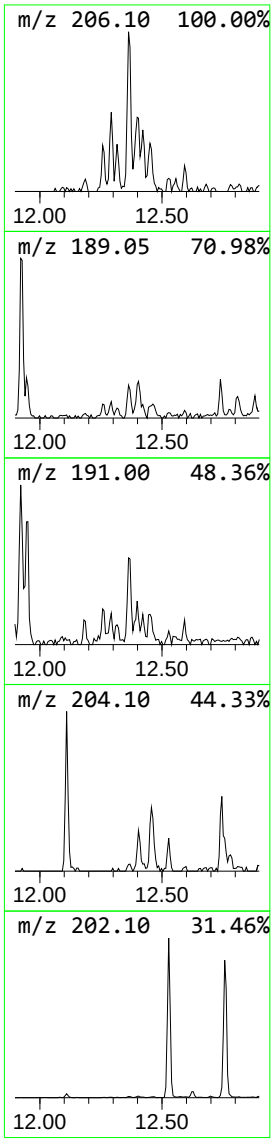
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	2.09 ng	37024	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	83
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	70
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	64
5	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

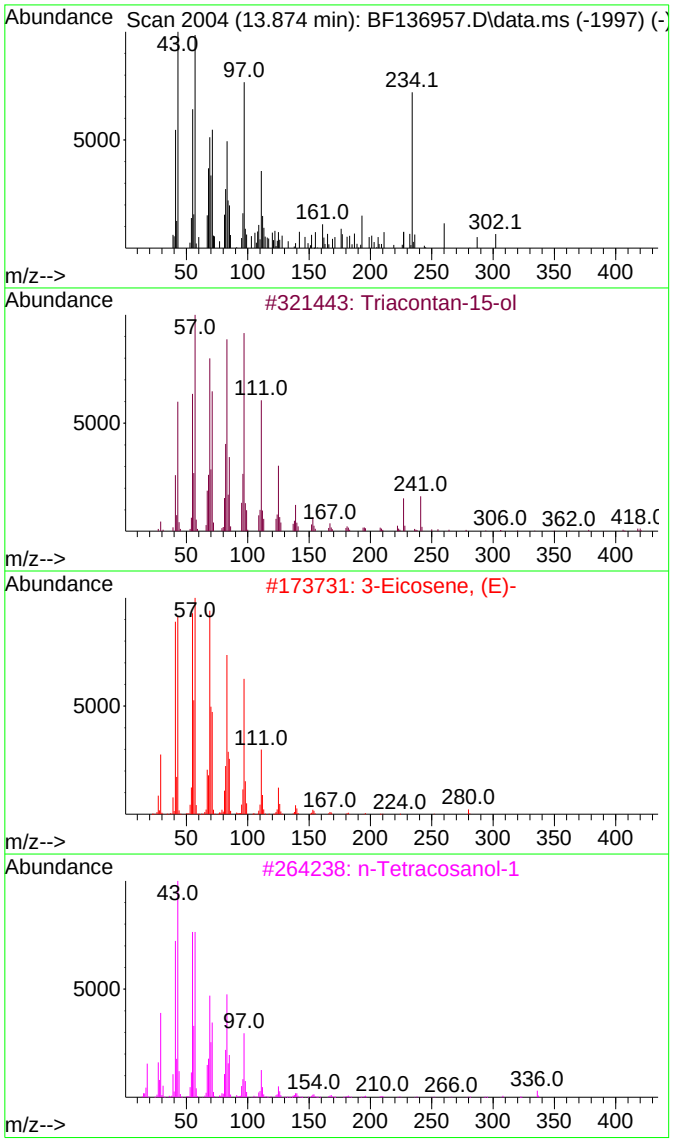
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

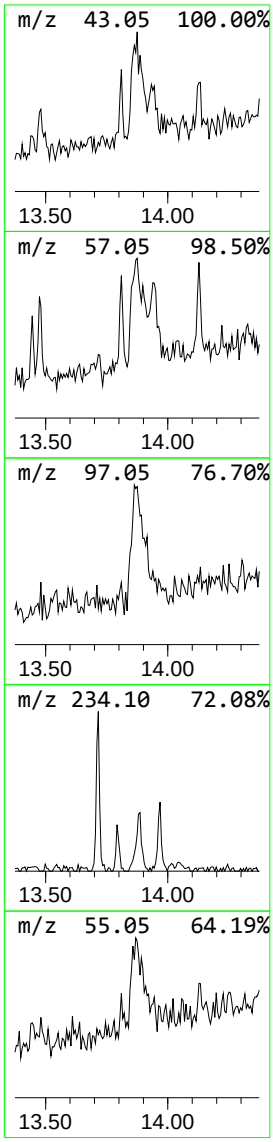
****

Peak Number 8 unknown13.874 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.55 ng	64714	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontan-15-ol	438	C30H62O	031849-26-0	43
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	38
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	38
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	30
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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

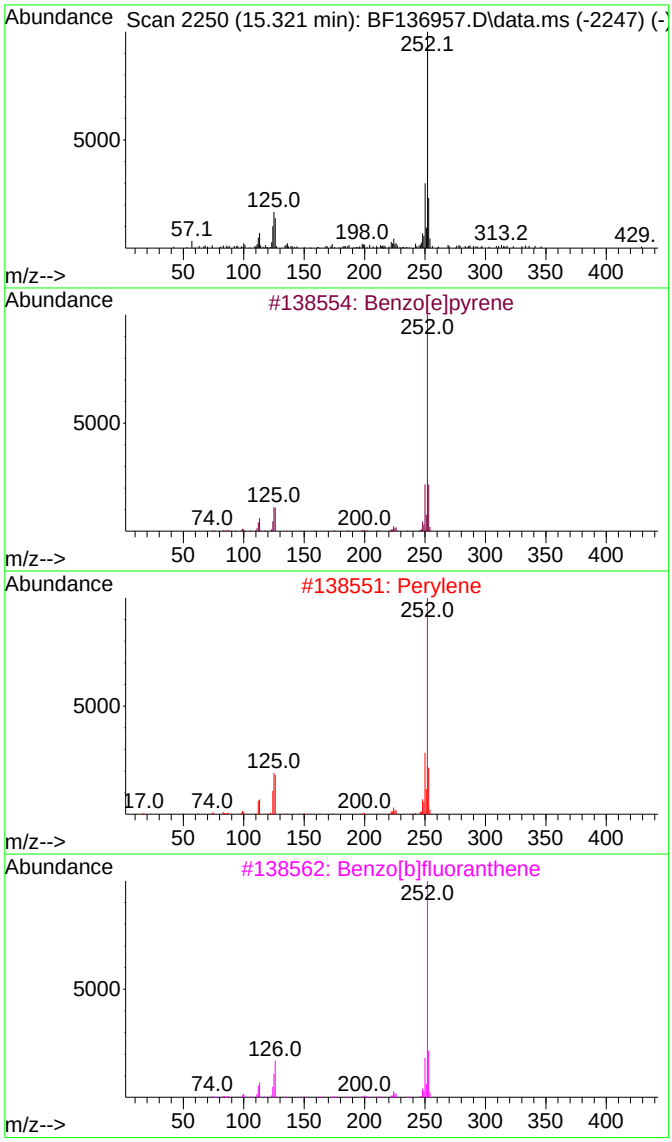
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

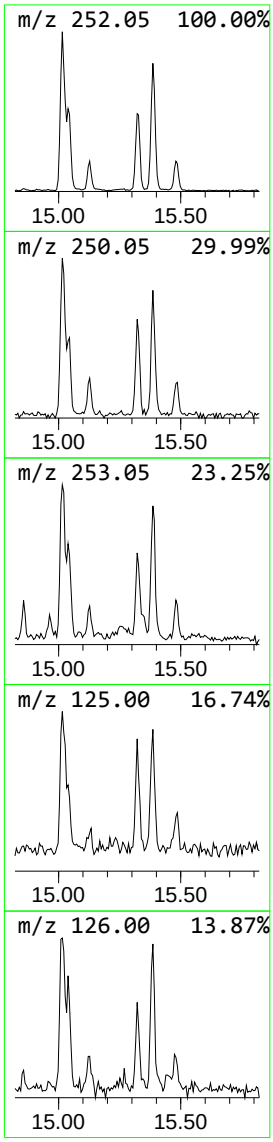
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	3.69 ng	54227	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136957.D
Acq On : 04 Jan 2024 23:54
Operator : CG\JU
Sample : 06015-07
Misc :
ALS Vial : 15 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
unknown5.004	5.004	2.2	ng	28665	1	6.781	264963	20.0
Phenanthrene, 2...	11.810	2.8	ng	48953	4	11.310	353661	20.0
Phenanthrene, 4...	11.839	8.4	ng	149163	4	11.310	353661	20.0
unknown11.922	11.922	4.6	ng	81912	4	11.310	353661	20.0
Phenanthrene, 2...	12.363	2.4	ng	42148	4	11.310	353661	20.0
Phenanthrene, 3...	12.398	2.1	ng	37024	4	11.310	353661	20.0
unknown13.874	13.874	2.5	ng	64714	5	13.969	508216	20.0
Benzo[e]pyrene	15.321	3.7	ng	54227	6	15.451	294170	20.0