LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139303.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	20	rVB	282836	433340	37.30%	3.195%
2	5.087	503	509	515	rBV	25504	33543	2.89%	0.247%
3	5.493	573	578	590	rVB	371506	464508	39.99%	3.425%
4	6.504	745	750	762	rBV	414032	504513	43.43%	3.720%
5	6.887	810	815	820	rVB	600653	720026	61.98%	5.309%
6	7.445	904	910	915	rBV	253355	320006	27.55%	2.359%
7	8.169	1027	1033	1040	rBV	744057	904653	77.88%	6.670%
8	9.239	1210	1215	1220	rBV	469973	580259	49.95%	4.278%
9	9.581	1268	1273	1276	rBV	11116	15268	1.31%	0.113%
10	9.787	1303	1308	1313	rBV	31050	39544	3.40%	0.292%
11	9.922	1326	1331	1336	rBV	747044	933627	80.37%	6.884%
12	10.128	1361	1366	1369	rBV	18425	23745	2.04%	0.175%
13	10.469	1420	1424	1430	rVB	37031	47788	4.11%	0.352%
14	10.634	1446	1452	1459	rVB	51555	70410	6.06%	0.519%
15	10.704	1459	1464	1470	rBV	217521	287136	24.72%	2.117%
16	10.828	1481	1485	1492	rBV5	12193	19452	1.67%	0.143%
17	11.016	1512	1517	1520	rBV3	15441	21884	1.88%	0.161%
18	11.145	1534	1539	1541	rBV3	10040	13552	1.17%	0.100%
19	11.210	1547	1550	1554	rVB	20574	25584	2.20%	0.189%
20	11.257	1554	1558	1563	rVV2	10980	20181	1.74%	0.149%
21	11.304	1563	1566	1571	rVB	14808	18327	1.58%	0.135%
22	11.410	1578	1584	1587	rBV	621673	928552	79.93%	6.846%
23	11.481	1592	1596	1600	rVV	67990	90492	7.79%	0.667%
24	11.516	1600	1602	1608	rVB3	10019	11684	1.01%	0.086%
25	11.639	1618	1623	1631	rBV3	9621	24529	2.11%	0.181%
26	11.704	1631	1634	1637	rVV2	13939	17776	1.53%	0.131%
27	11.739	1637	1640	1646	rVB6	11621	15760	1.36%	0.116%
28	11.910	1664	1669	1670	rBV	53536	60120	5.18%	0.443%
29	11.933	1670	1673	1678	rVV2	97374	139458	12.01%	1.028%
30	11.986	1678	1682	1684	rVV	22315	30021	2.58%	0.221%
31	12.022	1684	1688	1696	rVB	93250	165789	14.27%	1.222%
32	12.110	1696	1703	1706	rBV6	7865	15245	1.31%	0.112%
33	12.204	1715	1719	1721	rBV	29251	37996	3.27%	0.280%
34	12.357	1741	1745	1747	rBV2	10449	12288	1.06%	0.091%
35	12.386	1747	1750	1752	rVV	10013	11644	1.00%	0.086%
36	12.457	1757	1762	1765	rBV	34311	46740	4.02%	0.345%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.498	1765	1769	1773	rVV4	20176	39069	3.36%	0.288%
38	12.545	1773	1777	1783	rVB	40054	59802	5.15%	0.441%
39	12.622	1785	1790	1795	rBV	565748	699265	60.20%	5.156%
40	12.675	1795	1799	1803	rBV4	11113	21823	1.88%	0.161%
41	12.716	1803	1806	1809	rBV	15767	17286	1.49%	0.127%
42	12.851	1821	1829	1834	rBV	457488	673674	57.99%	4.967%
43	12.898	1834	1837	1842	rVB2	26313	36911	3.18%	0.272%
44	12.992	1844	1853	1860	rVB	338366	472964	40.71%	3.487%
45	13.069	1860	1866	1874	rBV3	49530	106632	9.18%	0.786%
46	13.175	1876	1884	1888	rVB3	65622	133018	11.45%	0.981%
47	13.245	1888	1896	1898	rBV	36454	58287	5.02%	0.430%
48	13.280	1898	1902	1909	rVV2	63243	96249	8.29%	0.710%
49	13.339	1909	1912	1914	rVV2	10452	13085	1.13%	0.096%
50	13.375	1914	1918	1920	rVV2	26211	35705	3.07%	0.263%
51	13.404	1920	1923	1932	rVV3	29931	51669	4.45%	0.381%
52	13.480	1933	1936	1941	rVV4	9866	15361	1.32%	0.113%
53	13.580	1945	1953	1959	rBV6	18838	57387	4.94%	0.423%
54	13.680	1966	1970	1975	rVB	62315	85448	7.36%	0.630%
55	13.792	1984	1989	1992	rBV2	52485	89349	7.69%	0.659%
56	13.827	1992	1995	1997	rVV	23616	29764	2.56%	0.219%
57	13.892	2002	2006	2012	rVB	69030	107312	9.24%	0.791%
58	14.045	2025	2032	2036	rBV2	651072	1161646	100.00%	8.565%
59	14.151	2048	2050	2053	rVB	13548	12321	1.06%	0.091%
60	14.186	2053	2056	2061	rBV2	22771	38943	3.35%	0.287%
61	14.433	2094	2098	2101	rVB	42433	50785	4.37%	0.374%
62	14.469	2101	2104	2107	rVB2	34643	40765	3.51%	0.301%
63	14.521	2109	2113	2116	rBV4	37512	61686	5.31%	0.455%
64	14.910	2176	2179	2187	rBV3	18841	41741	3.59%	0.308%
65	14.980	2188	2191	2197	rVB3	24673	43320	3.73%	0.319%
66	15.092	2204	2210	2219	rBV	224575	531166	45.73%	3.916%
67	15.174	2220	2224	2227	rBV2	79123	124694	10.73%	0.919%
68	15.398	2257	2262	2267	rVB	105948	166408	14.33%	1.227%
69	15.457	2267	2272	2278	rVV	157628	237836	20.47%	1.754%
70	15.521	2278	2283	2296	rVB2	306749	554923	47.77%	4.091%
71	15.768	2321	2325	2330	rVB2	30708	45963	3.96%	0.339%
72	16.004	2361	2365	2371	rVB	70038	110876	9.54%	0.817%
73	16.821	2499	2504	2513	rVB4	30071	71924	6.19%	0.530%
74	16.998	2528	2534	2543	rVB2	65737	146930	12.65%	1.083%
75	17.439	2603	2609	2622	rVB	49316	115752	9.96%	0.853%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

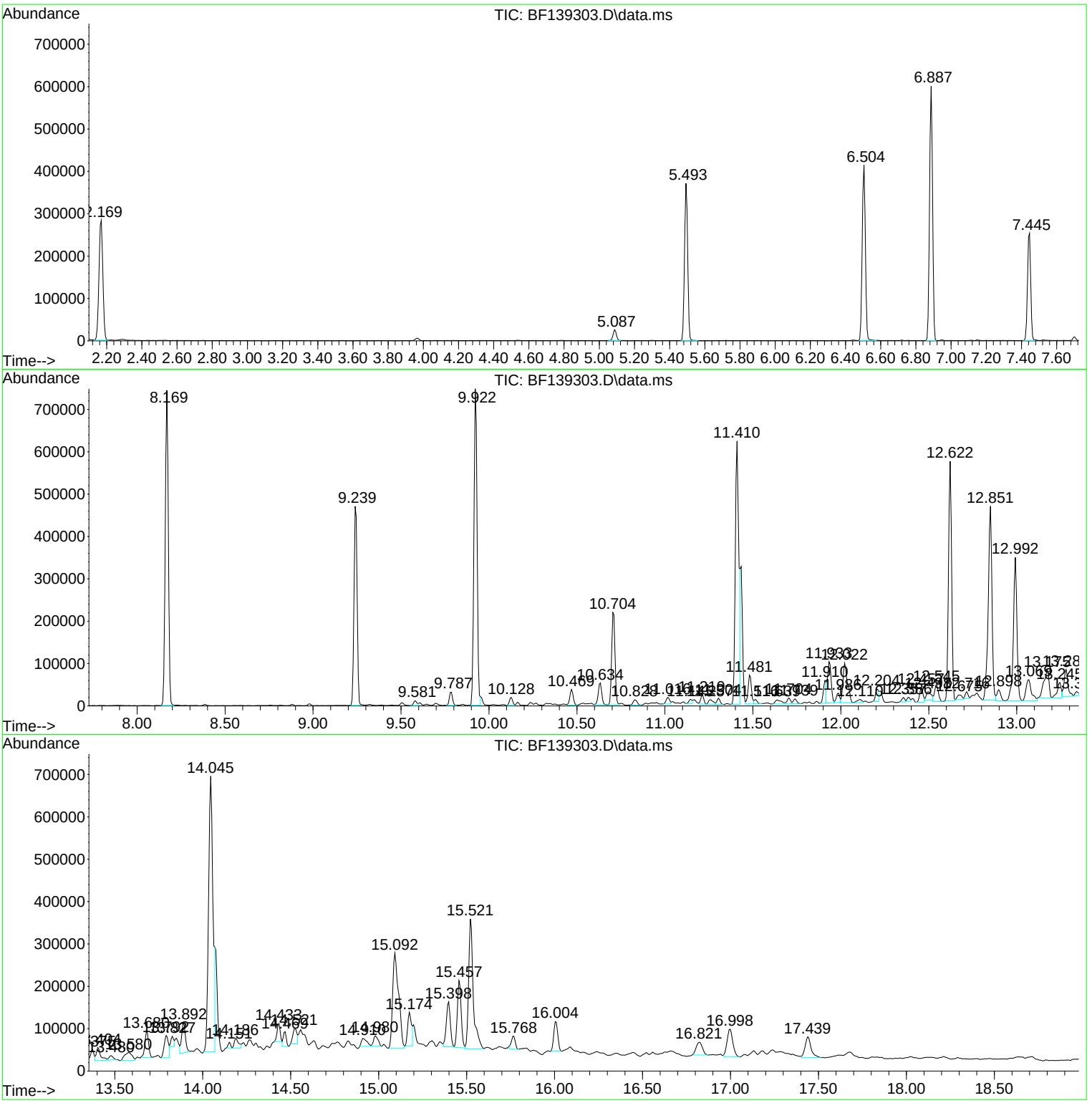
Sum of corrected areas: 13563179

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

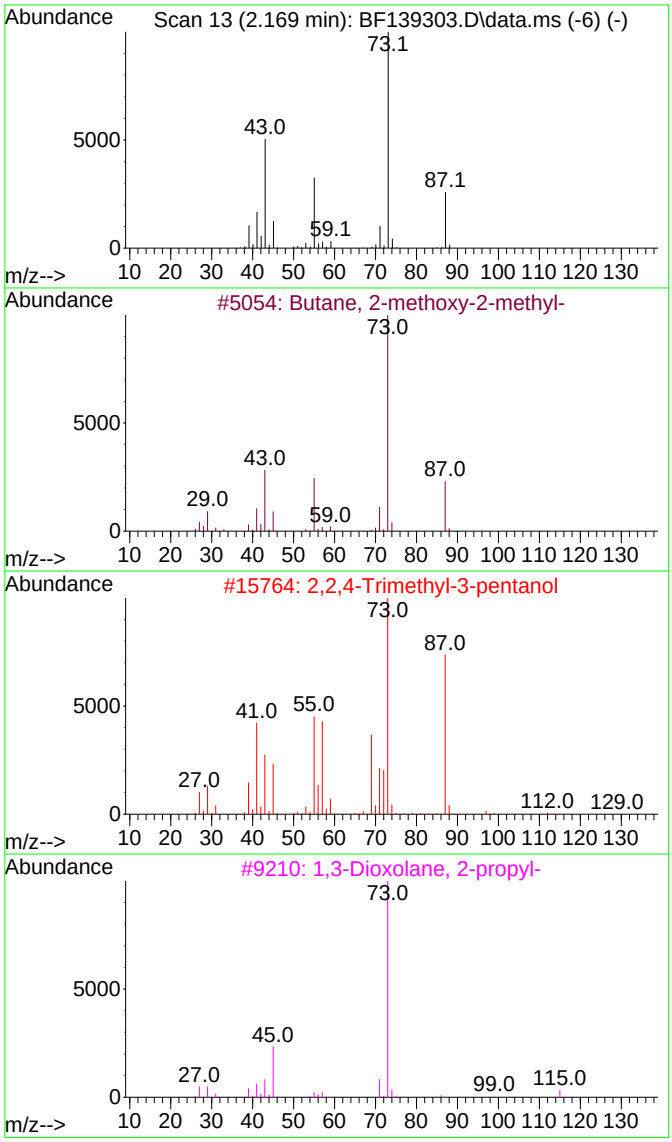
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

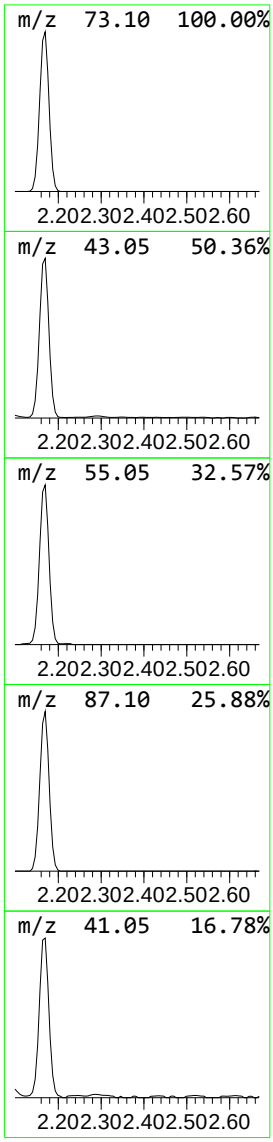
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	12.04 ng	433340	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

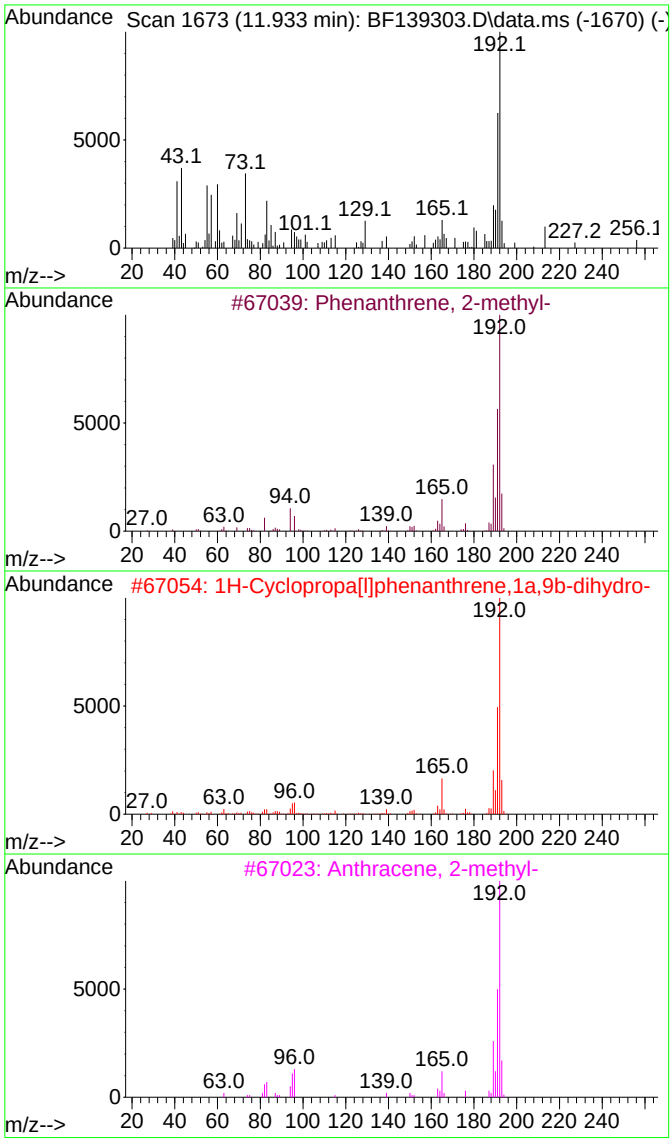
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

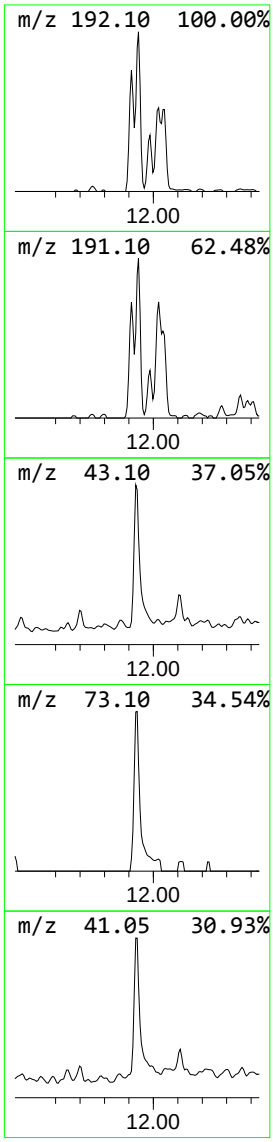
****

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.00 ng	139458	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	64
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

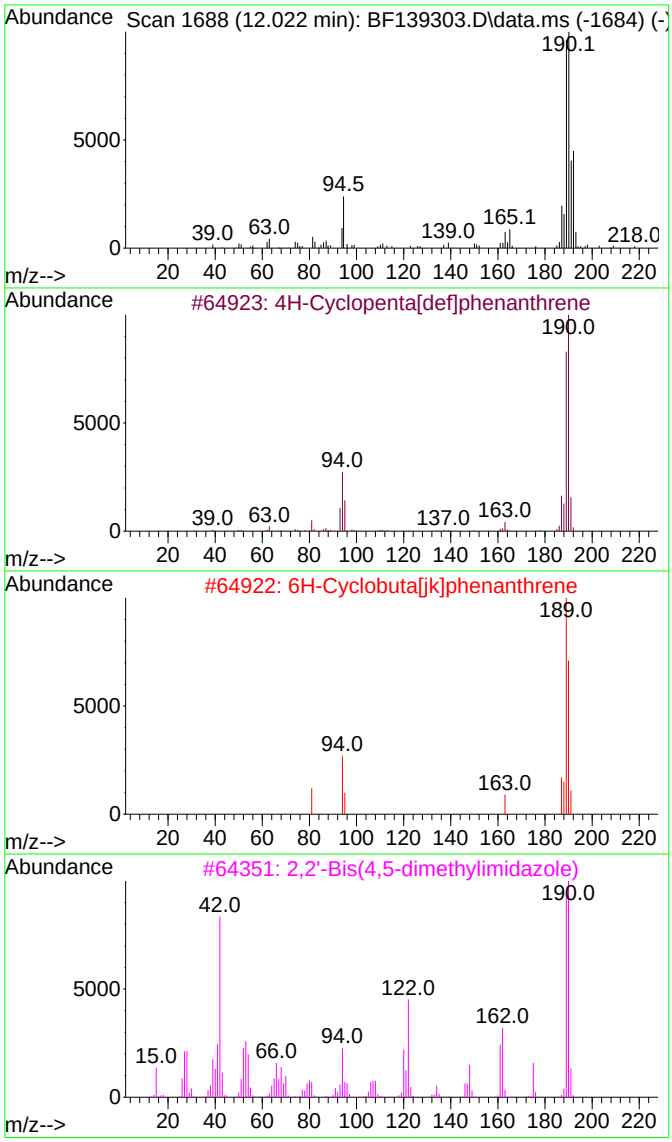
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

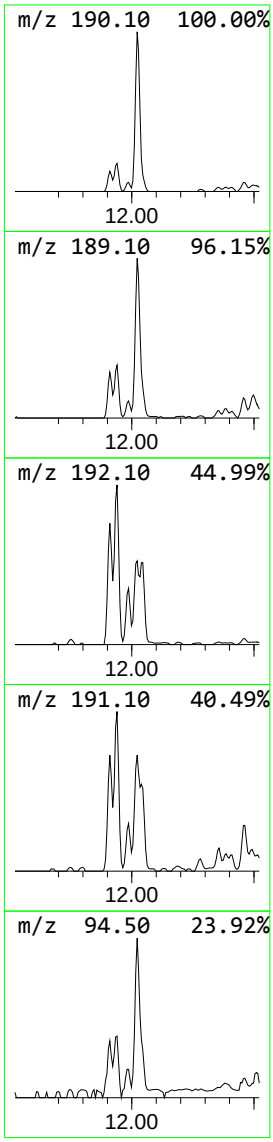
****

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	3.57 ng	165789	Phenanthrene-d10	11.410

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	42
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	Methyl diselenide	190	C2H6Se2	007101-31-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

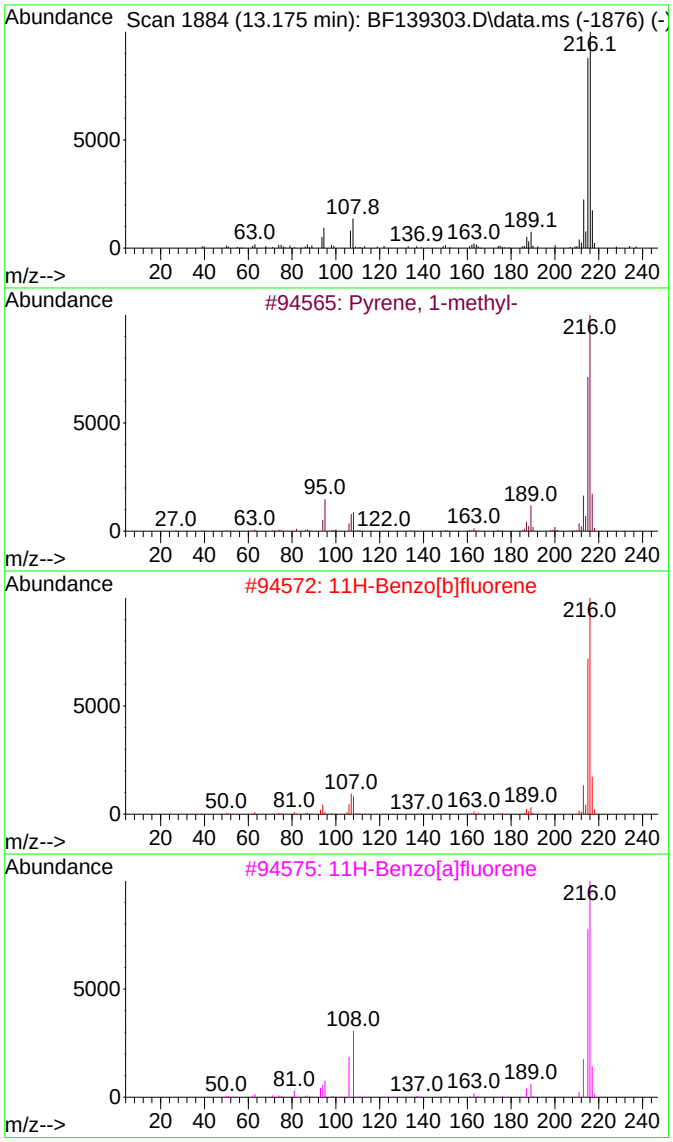
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

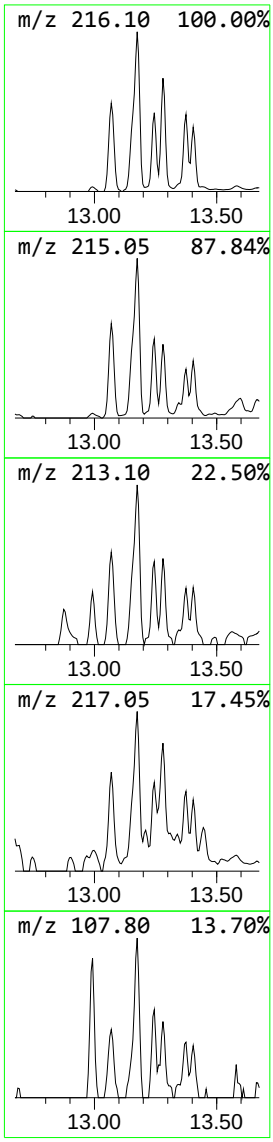
****

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.175	2.29 ng	133018	Chrysene-d12	14.045

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	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

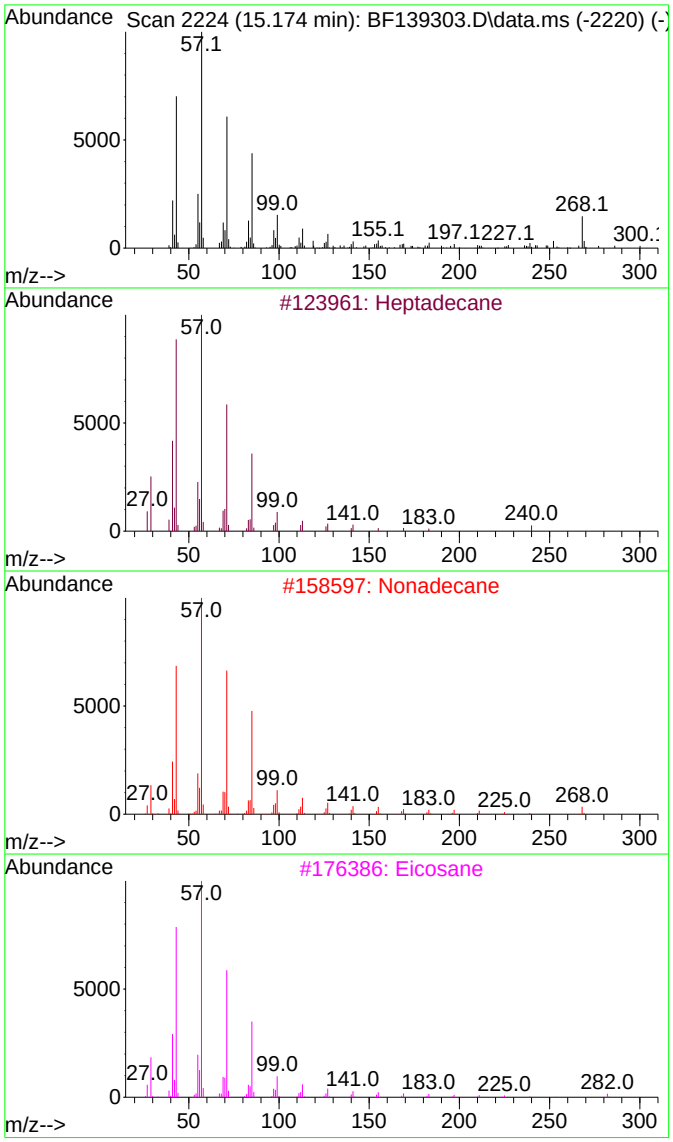
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

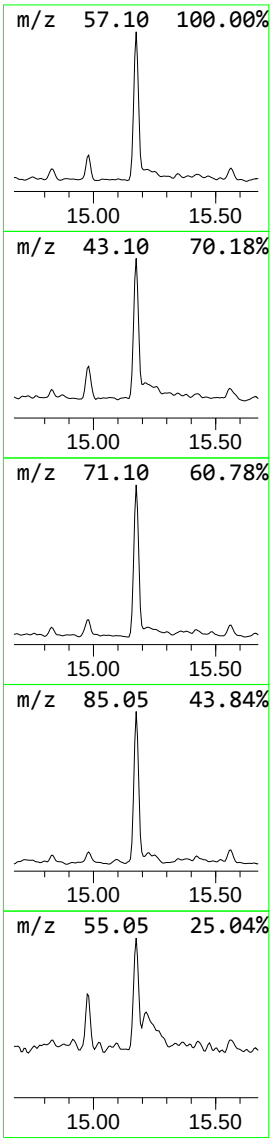
****

Peak Number 5 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	4.49 ng	124694	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Nonadecane	268	C19H40	000629-92-5	93
3	Eicosane	282	C20H42	000112-95-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

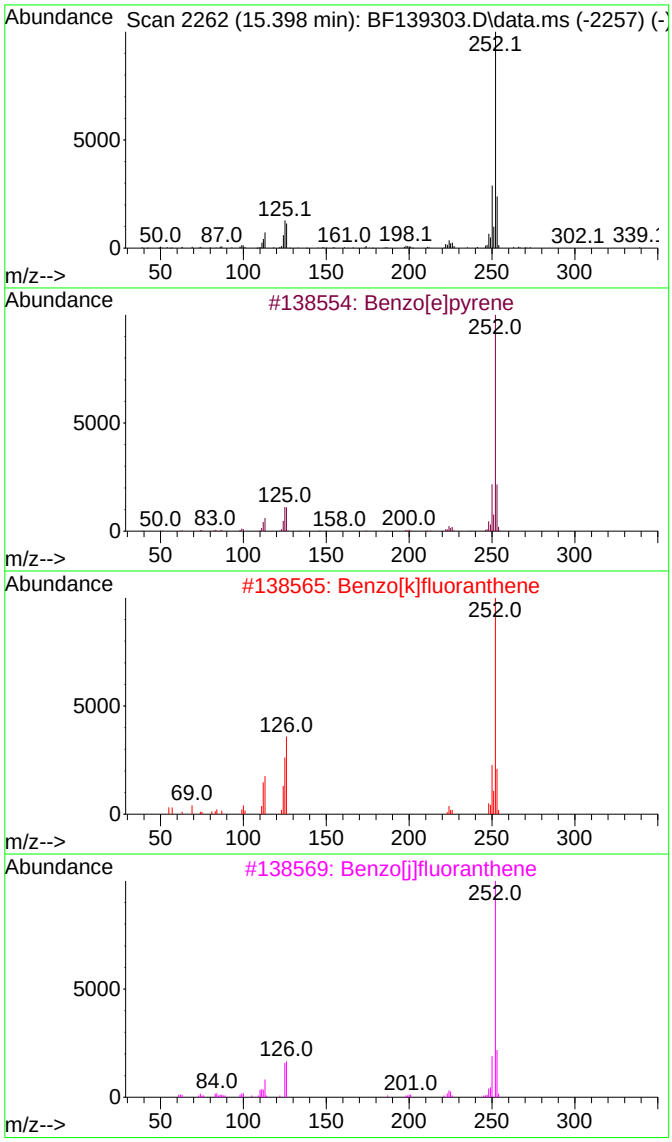
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

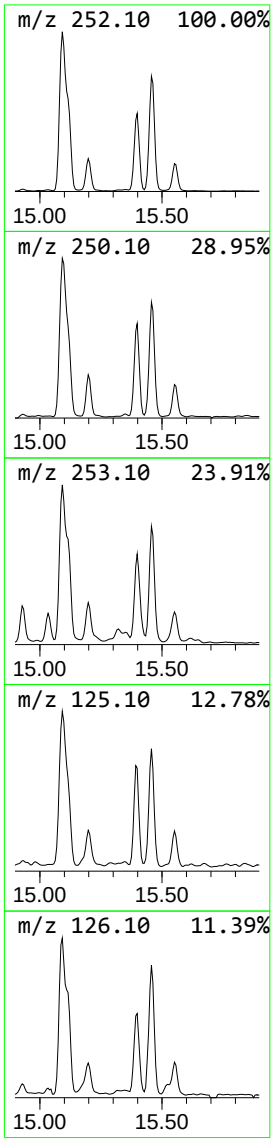
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	6.00 ng	166408	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

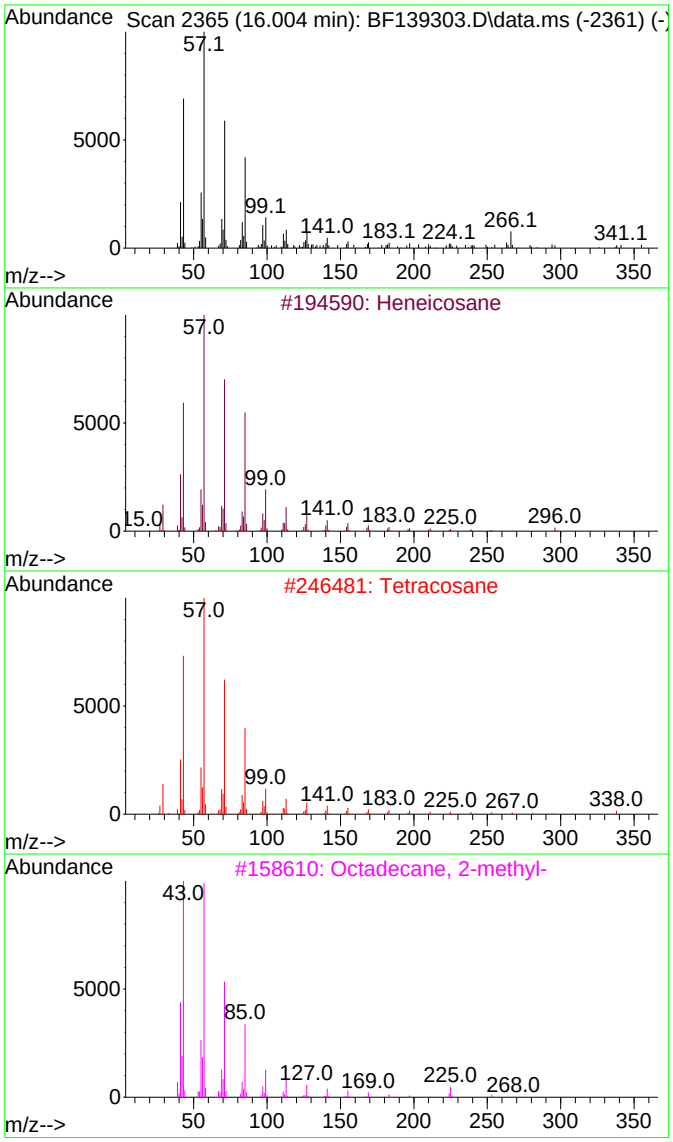
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

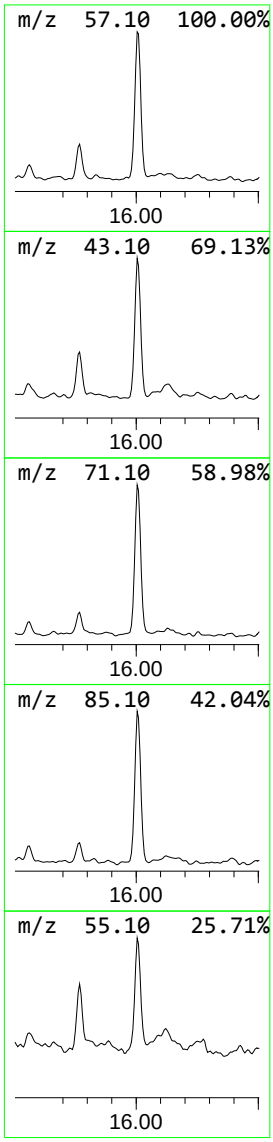
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	4.00 ng	110876	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Tetracosane	338	C24H50	000646-31-1	98
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	91
5	Heptacosane	380	C27H56	000593-49-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

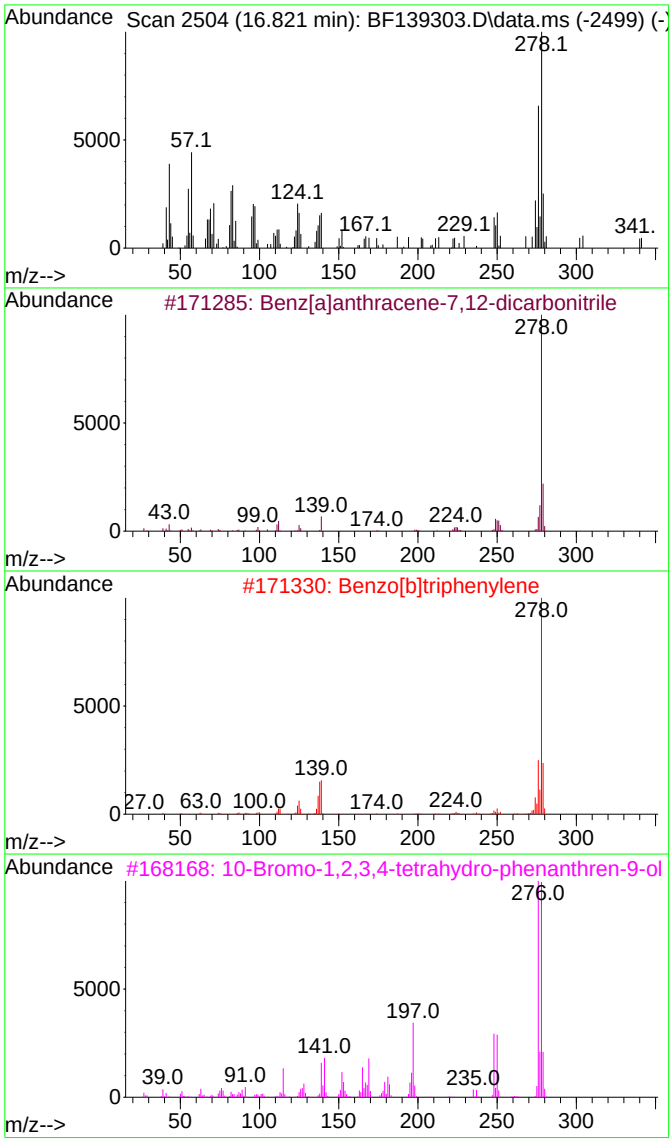
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

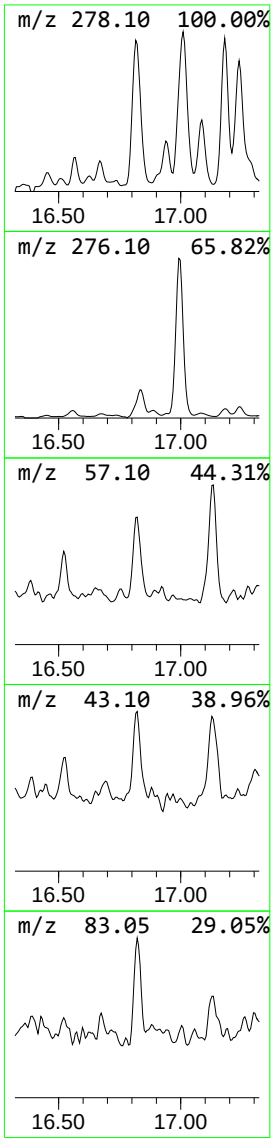
****

Peak Number 8 Benz[a]anthracene-7,12-dica... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.821	2.59 ng	71924	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	78
2	Benzo[b]triphenylene	278	C22H14	000215-58-7	55
3	10-Bromo-1,2,3,4-tetrahydro-phen...	276	C14H13BrO	1000190-54-9	53
4	Picene	278	C22H14	000213-46-7	50
5	Pyridine-3-carbonitrile, 2-oxo-4...	278	C16H10N2OS	1000304-72-3	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139303.D
Acq On : 10 Sep 2024 16:58
Operator : RC/JU
Sample : P3906-07 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-701-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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
Butane, 2-metho...	2.169	12.0	ng	433340	1	6.887	720026	20.0
Phenanthrene, 2...	11.933	3.0	ng	139458	4	11.410	928552	20.0
4H-Cyclopenta[d...	12.022	3.6	ng	165789	4	11.410	928552	20.0
Pyrene, 1-methyl-	13.175	2.3	ng	133018	5	14.045	1161650	20.0
Heptadecane	15.174	4.5	ng	124694	6	15.521	554923	20.0
Benzo[e]pyrene	15.398	6.0	ng	166408	6	15.521	554923	20.0
Heneicosane	16.004	4.0	ng	110876	6	15.521	554923	20.0
Benz[a]anthrace...	16.821	2.6	ng	71924	6	15.521	554923	20.0