LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141928.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	13	rVB	242181	335161	20.33%	2.163%
2	2.334	34	41	50	rVB	53959	91882	5.57%	0.593%
3	5.487	572	577	588	rBV	313989	415203	25.18%	2.679%
4	6.440	734	739	743	rBV	10040	16834	1.02%	0.109%
5	6.493	743	748	761	rVB	321552	428811	26.01%	2.767%
6	6.881	809	814	819	rBV	593587	729225	44.22%	4.706%
7	7.434	903	908	919	rBV	200696	260869	15.82%	1.683%
8	8.157	1026	1031	1040	rBV	696469	930757	56.45%	6.006%
9	9.228	1208	1213	1223	rBV	430159	558128	33.85%	3.602%
10	9.569	1267	1271	1274	rBV	12825	17253	1.05%	0.111%
11	9.775	1301	1306	1310	rBV	21434	26719	1.62%	0.172%
12	9.910	1324	1329	1334	rBV	777308	1002280	60.78%	6.468%
13	9.945	1334	1335	1339	rVB	31681	22760	1.38%	0.147%
14	10.116	1359	1364	1367	rBV	28570	36560	2.22%	0.236%
15	10.228	1378	1383	1386	rBV3	11988	17935	1.09%	0.116%
16	10.316	1393	1398	1405	rBV5	9232	21874	1.33%	0.141%
17	10.457	1418	1422	1427	rVB	41557	54550	3.31%	0.352%
18	10.622	1444	1450	1457	rVB	67928	90883	5.51%	0.586%
19	10.698	1458	1463	1475	rVB2	256235	351630	21.32%	2.269%
20	10.822	1479	1484	1490	rVB3	20642	34464	2.09%	0.222%
21	11.010	1509	1516	1519	rBV3	19562	36952	2.24%	0.238%
22	11.133	1532	1537	1539	rBV2	21952	32160	1.95%	0.208%
23	11.245	1552	1556	1561	rVV2	19165	33052	2.00%	0.213%
24	11.298	1561	1565	1569	rVB	15604	23897	1.45%	0.154%
25	11.398	1577	1582	1590	rBV2	777309	1320639	80.09%	8.522%
26	11.475	1590	1595	1598	rVV	91562	129183	7.83%	0.834%
27	11.504	1598	1600	1607	rVB2	12994	18508	1.12%	0.119%
28	11.628	1617	1621	1623	rBV	19402	26966	1.64%	0.174%
29	11.692	1629	1632	1636	rVV	17393	21716	1.32%	0.140%
30	11.728	1636	1638	1644	rVB5	14138	17857	1.08%	0.115%
31	11.922	1668	1671	1676	rVB2	111651	168503	10.22%	1.087%
32	11.975	1676	1680	1683	rVV2	30098	40132	2.43%	0.259%
33	12.010	1683	1686	1694	rVB	119094	227319	13.79%	1.467%
34	12.092	1696	1700	1704	rBV6	10372	19464	1.18%	0.126%
35	12.198	1713	1718	1727	rVB2	47675	98323	5.96%	0.634%
36	12.345	1737	1743	1745	rBV2	26650	40829	2.48%	0.263%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.375	1745	1748	1750	rVV	17752	18693	1.13%	0.121%
38	12.451	1756	1761	1764	rBV	71754	109742	6.66%	0.708%
39	12.486	1764	1767	1772	rVV2	43990	80784	4.90%	0.521%
40	12.533	1772	1775	1783	rVB	54844	80526	4.88%	0.520%
41	12.610	1783	1788	1793	rBV	740321	916385	55.58%	5.913%
42	12.675	1793	1799	1801	rBV3	17004	35144	2.13%	0.227%
43	12.704	1801	1804	1807	rVV	18648	19951	1.21%	0.129%
44	12.839	1820	1827	1833	rBV	656628	982230	59.57%	6.338%
45	12.886	1833	1835	1840	rVB2	33078	43212	2.62%	0.279%
46	12.980	1843	1851	1858	rVB	471442	673847	40.87%	4.348%
47	13.057	1858	1864	1871	rBV4	79210	160351	9.72%	1.035%
48	13.163	1875	1882	1887	rVB	109839	214660	13.02%	1.385%
49	13.233	1890	1894	1897	rBV2	62737	81759	4.96%	0.528%
50	13.269	1897	1900	1904	rVB2	78853	94330	5.72%	0.609%
51	13.363	1913	1916	1918	rBV	38432	41592	2.52%	0.268%
52	13.392	1919	1921	1925	rVB	36028	41485	2.52%	0.268%
53	13.669	1965	1968	1976	rVB	62973	93638	5.68%	0.604%
54	13.786	1983	1988	1990	rBV2	56122	96578	5.86%	0.623%
55	13.816	1990	1993	1995	rVV	31704	40001	2.43%	0.258%
56	13.880	2001	2004	2013	rVB2	93803	144519	8.76%	0.933%
57	14.033	2024	2030	2034	rBV2	972126	1648915	100.00%	10.640%
58	14.139	2046	2048	2052	rVB	38008	39275	2.38%	0.253%
59	14.198	2056	2058	2064	rVB4	59607	81703	4.95%	0.527%
60	14.421	2093	2096	2099	rVB	55539	61748	3.74%	0.398%
61	14.510	2107	2111	2114	rBV3	87505	130134	7.89%	0.840%
62	14.816	2160	2163	2166	rVB2	53711	62031	3.76%	0.400%
63	15.080	2203	2208	2216	rVB	251570	570041	34.57%	3.678%
64	15.380	2255	2259	2265	rVB	124969	195182	11.84%	1.259%
65	15.445	2265	2270	2275	rBV	182788	278567	16.89%	1.798%
66	15.510	2276	2281	2285	rBV	367356	596431	36.17%	3.849%
67	16.986	2528	2532	2542	rVB2	81809	164146	9.95%	1.059%

Sum of corrected areas: 15496878

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
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Acq On : 11 Mar 2025 21:12
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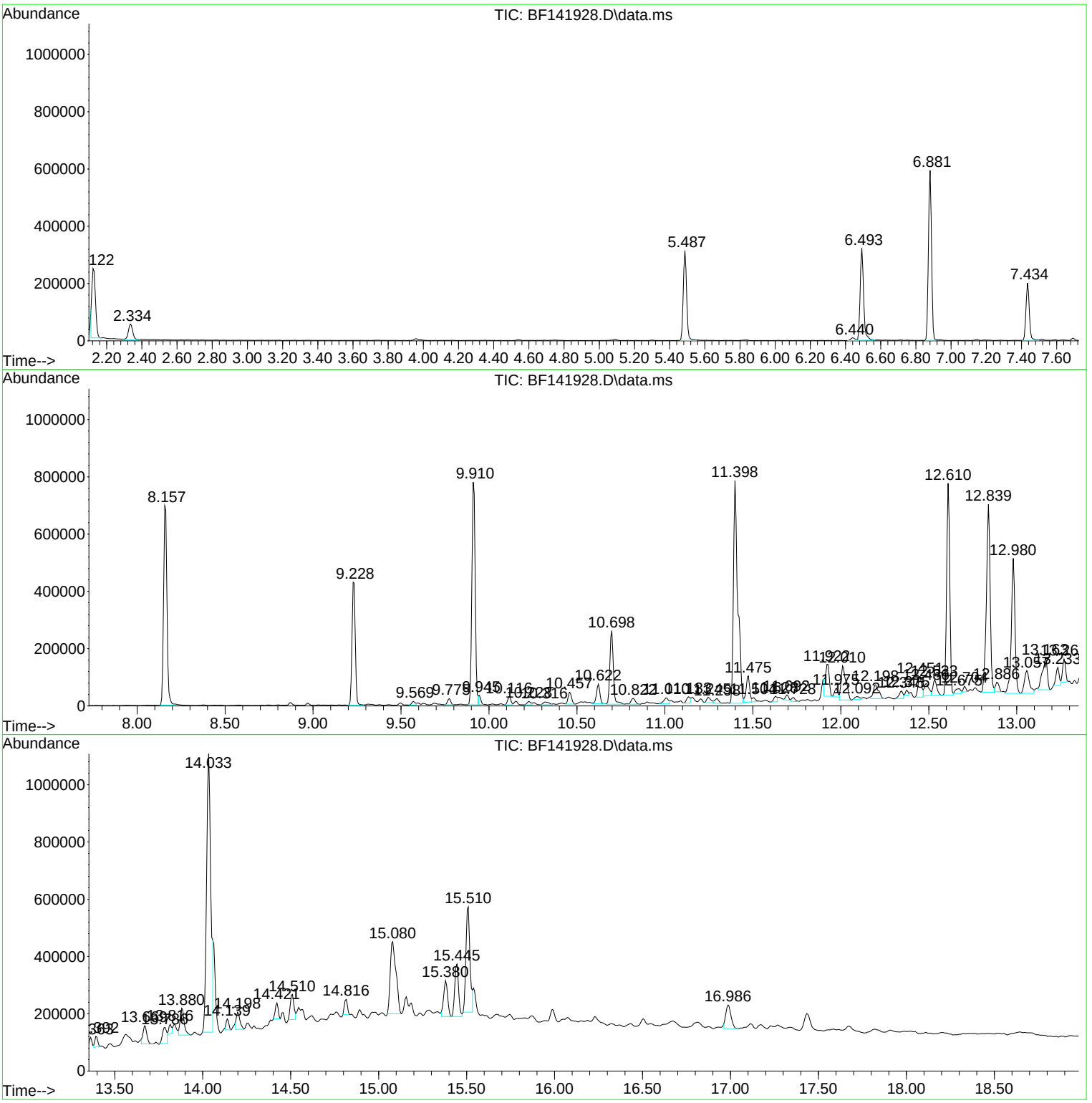
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

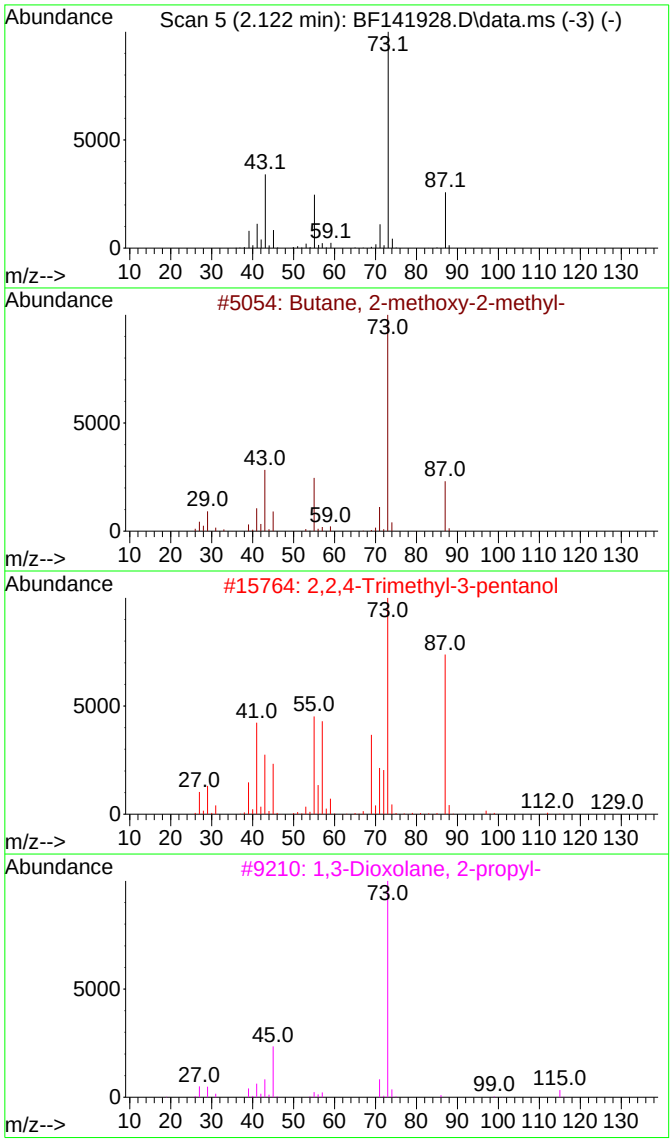
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

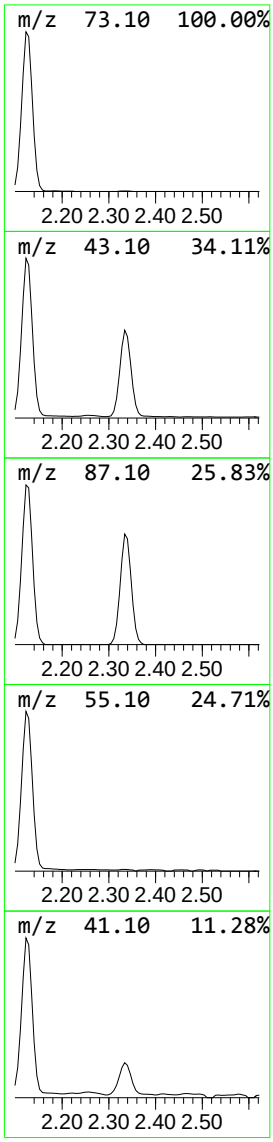
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	9.19 ng	335161	1,4-Dichlorobenzene-d4	6.881

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

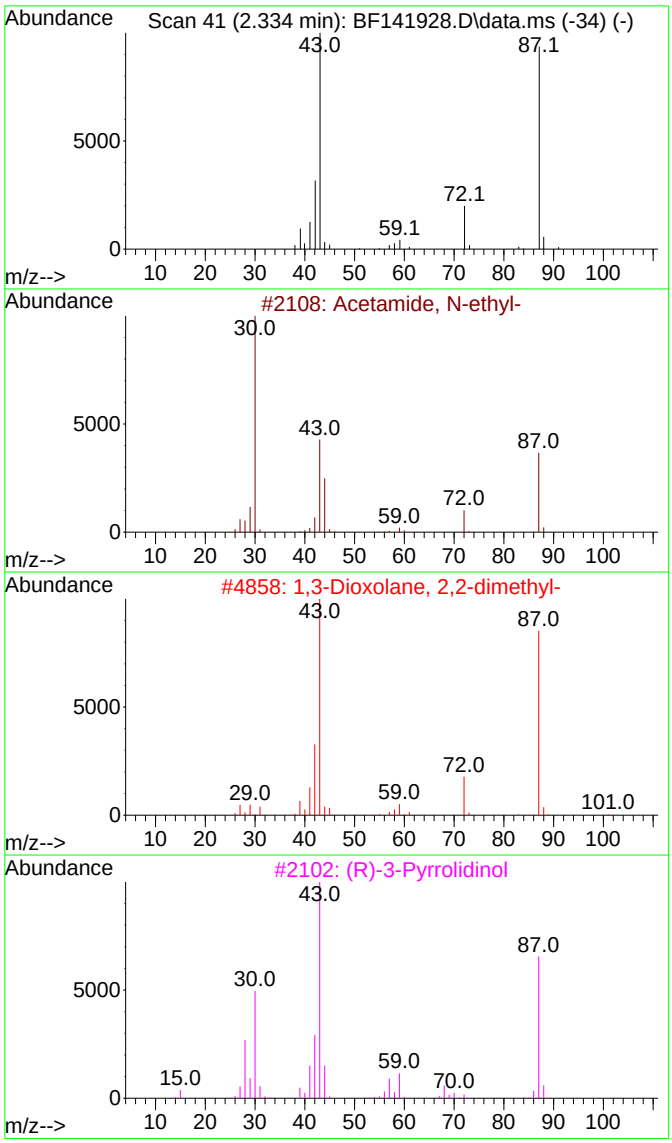
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

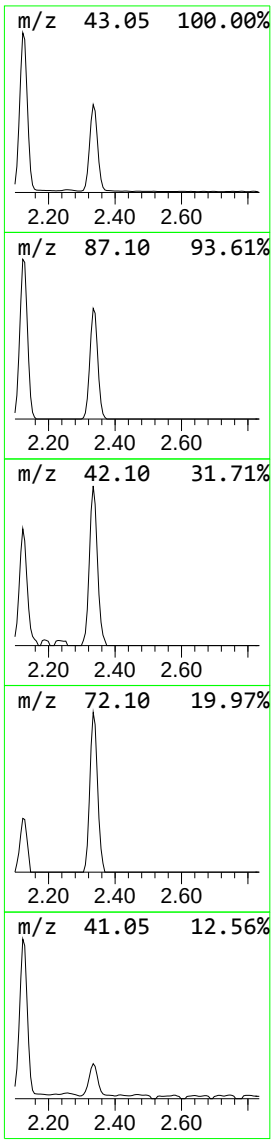
****

Peak Number 2 Acetamide, N-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	2.52 ng	91882	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	78
2	1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	64
3	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	39
4	2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	38
5	N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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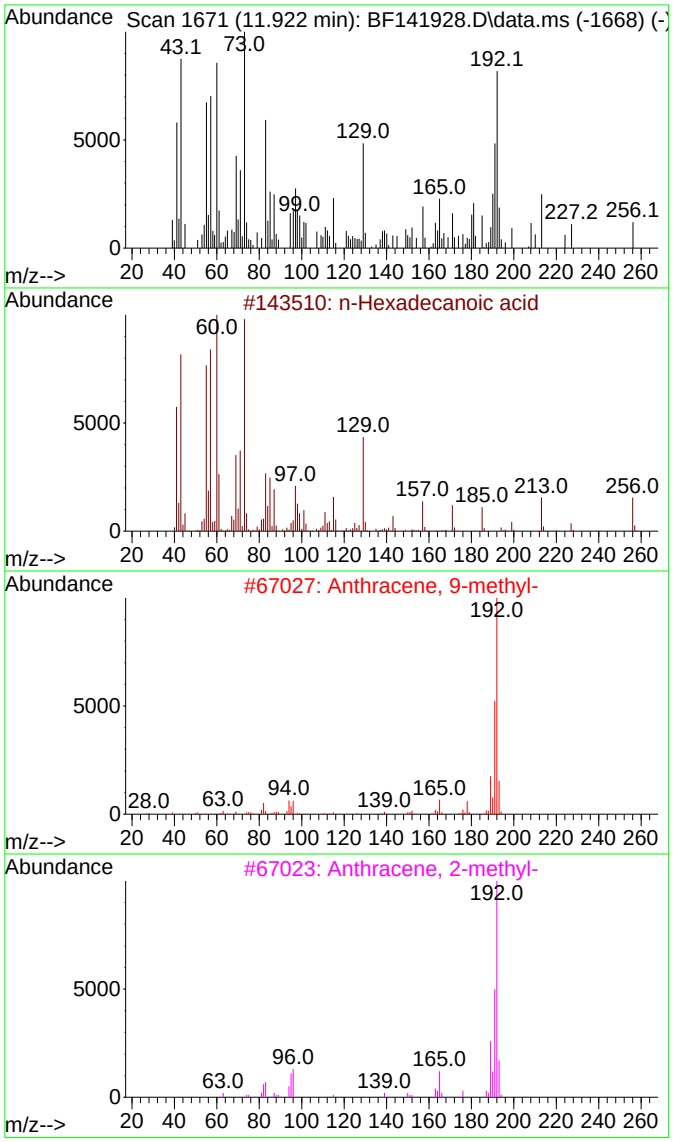
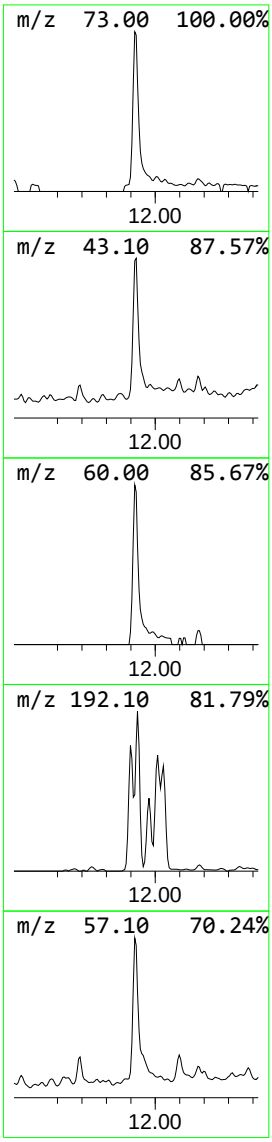
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.55 ng	168503	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	49
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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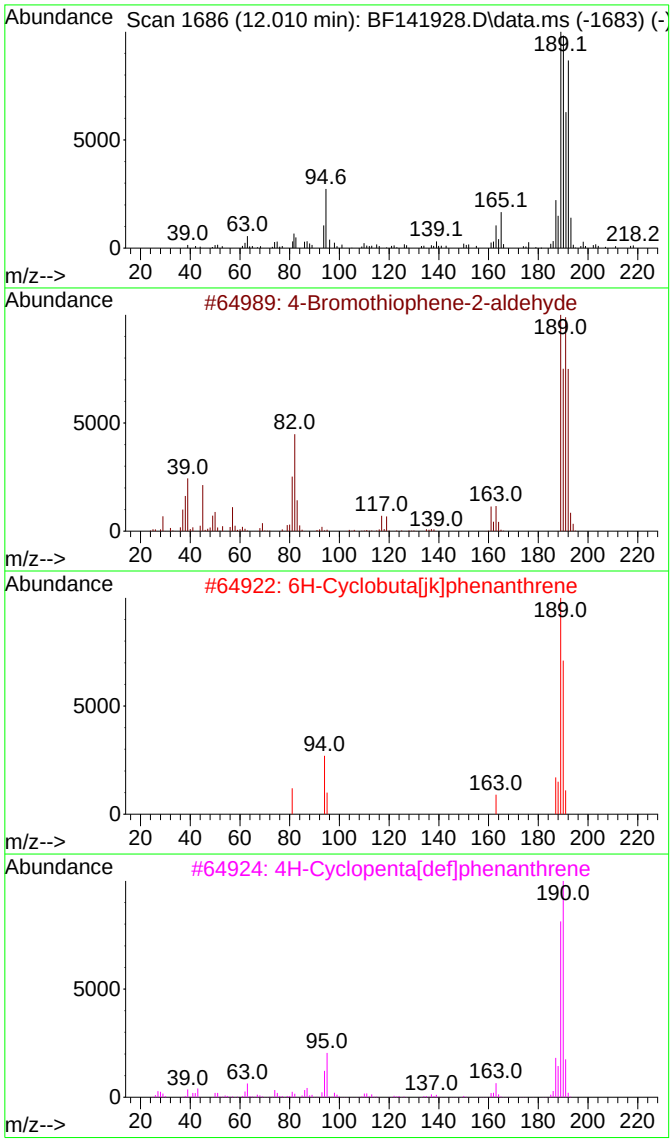
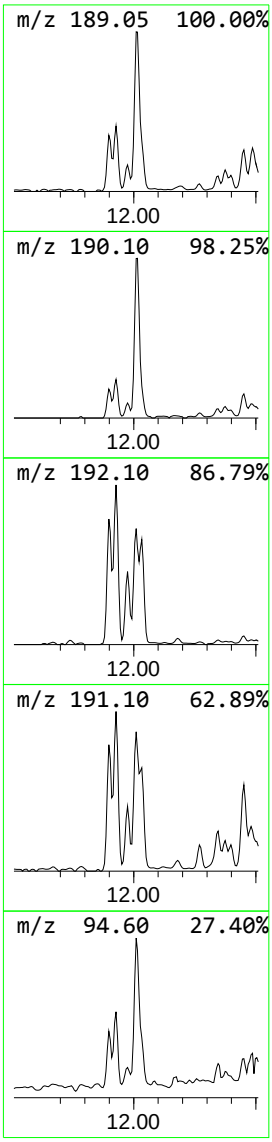
Peak Number 4 4-Bromothiophene-2-aldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	3.44 ng	227319	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	58
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

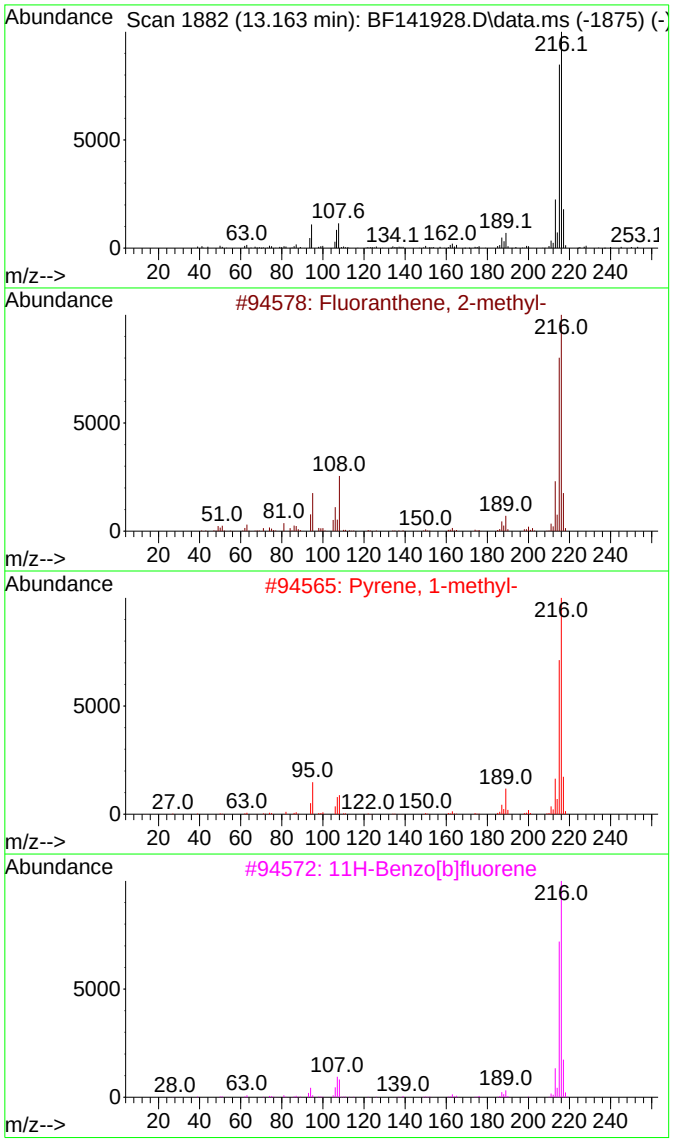
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

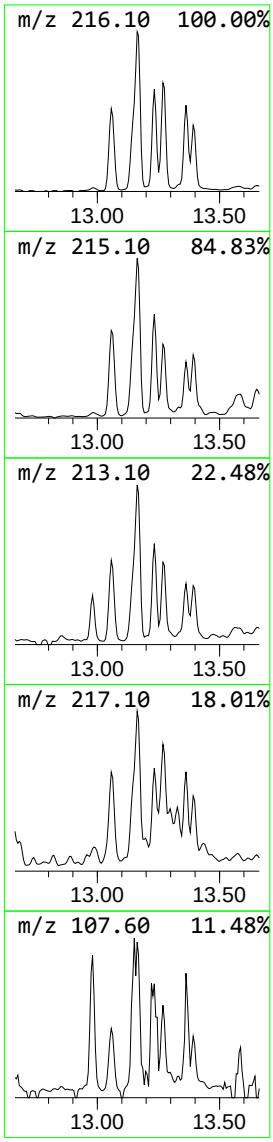
****

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.60 ng	214660	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

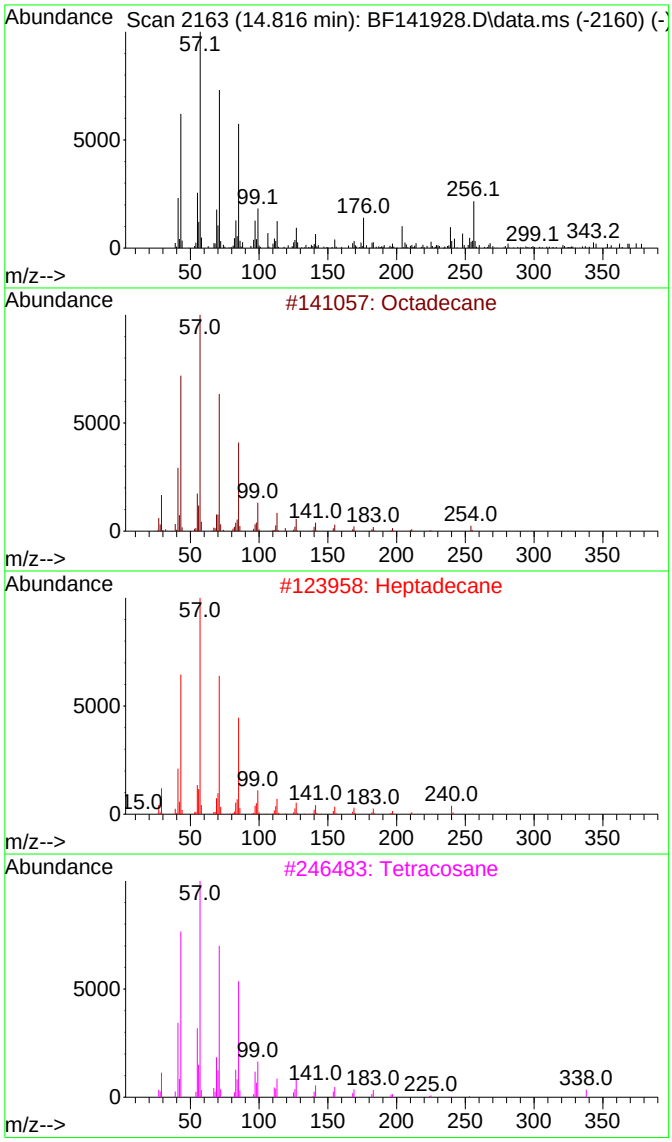
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

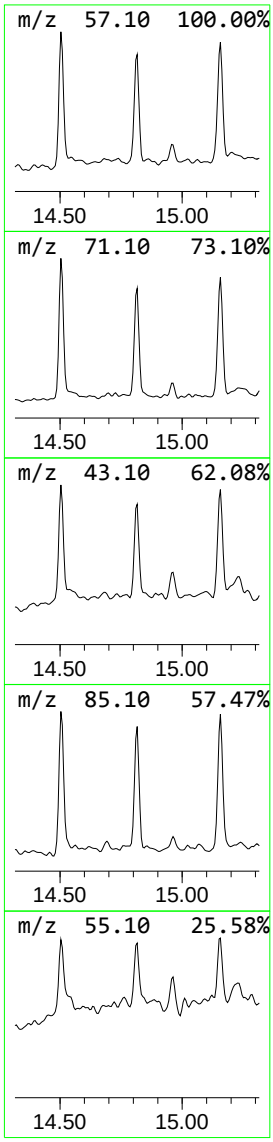
****

Peak Number 6 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.08 ng	62031	Perylene-d12	15.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Heptadecane	240	C17H36	000629-78-7	86
3	Tetracosane	338	C24H50	000646-31-1	78
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
5	Hexacosane	366	C26H54	000630-01-3	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

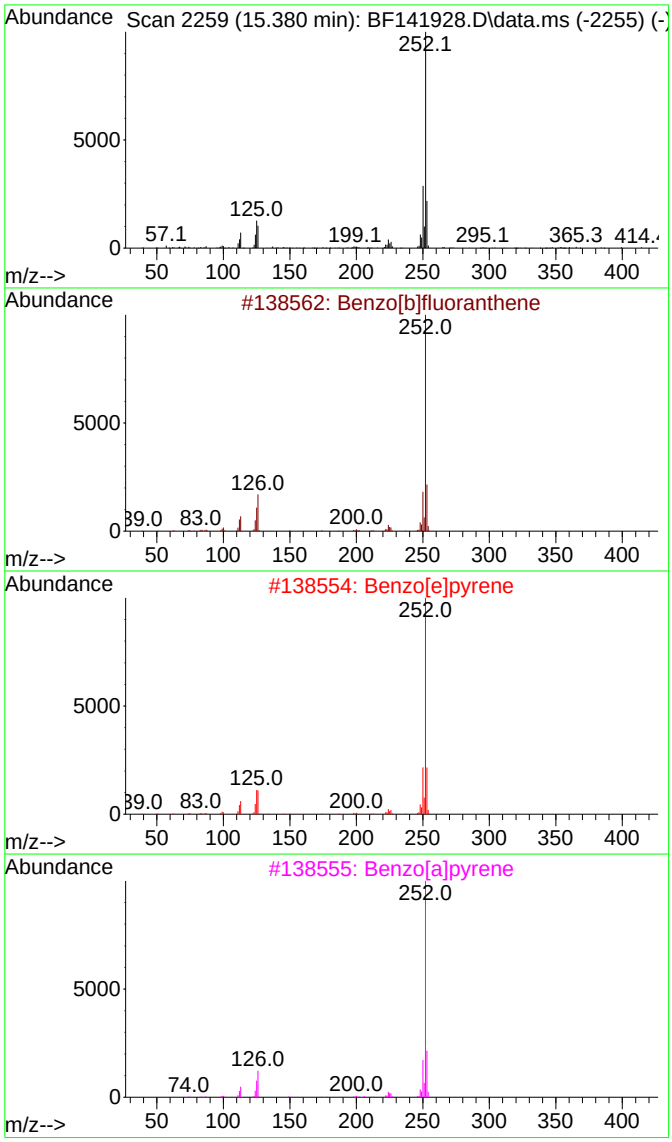
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

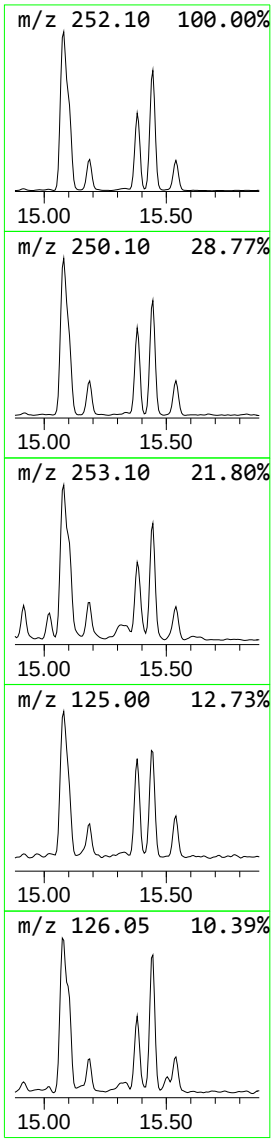
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	6.54 ng	195182	Perylene-d12	15.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141928.D
Acq On : 11 Mar 2025 21:12
Operator : RC/JU
Sample : Q1535-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-03102025

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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...	2.122	9.2	ng	335161	1	6.881	729225	20.0
Acetamide, N-et...	2.334	2.5	ng	91882	1	6.881	729225	20.0
n-Hexadecanoic ...	11.922	2.5	ng	168503	4	11.398	1320640	20.0
4-Bromothiophen...	12.010	3.4	ng	227319	4	11.398	1320640	20.0
Fluoranthene, 2...	13.163	2.6	ng	214660	5	14.033	1648920	20.0
Octadecane	14.816	2.1	ng	62031	6	15.510	596431	20.0
Benzo[e]pyrene	15.380	6.5	ng	195182	6	15.510	596431	20.0