LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124981.D
Acq On : 7 Aug 2021 18:58
Operator : JU/CG
Sample : M3289-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	16	18	20	rBB	2083	1921	1.47%	0.134%
2	5.045	498	503	507	rBB	58217	69619	53.18%	4.840%
3	5.451	568	572	575	rBB	127297	122165	93.31%	8.493%
4	5.839	636	638	641	rBB	13771	10926	8.35%	0.760%
5	6.463	739	744	747	rBB	135398	128817	98.39%	8.955%
6	6.828	803	806	809	rBB	43769	30764	23.50%	2.139%
7	6.892	814	817	823	rBB	1717	2346	1.79%	0.163%
8	7.392	898	902	905	rBB	96977	79611	60.81%	5.535%
9	8.010	1004	1007	1010	rBV	44589	36356	27.77%	2.527%
10	8.110	1021	1024	1027	rBB	59183	43098	32.92%	2.996%
11	9.186	1203	1207	1210	rBB	173955	130923	100.00%	9.102%
12	9.863	1319	1322	1325	rBB	70659	52390	40.02%	3.642%
13	10.651	1453	1456	1459	rBB	110244	90184	68.88%	6.270%
14	11.351	1572	1575	1577	rBV	68604	51885	39.63%	3.607%
15	11.374	1577	1579	1582	rVB	47503	33981	25.95%	2.362%
16	11.427	1585	1588	1590	rBB	6715	5052	3.86%	0.351%
17	11.580	1612	1614	1616	rBB	3086	1999	1.53%	0.139%
18	11.851	1658	1660	1662	rBV	3136	2916	2.23%	0.203%
19	11.874	1662	1664	1667	rVB3	6185	5616	4.29%	0.390%
20	11.927	1670	1673	1675	rBV3	1285	1715	1.31%	0.119%
21	11.963	1677	1679	1681	rBV	6353	5318	4.06%	0.370%
22	12.145	1706	1710	1712	rVB	3179	2610	1.99%	0.181%
23	12.563	1778	1781	1785	rVB	89237	74359	56.80%	5.169%
24	12.792	1814	1820	1824	rBB	66904	64401	49.19%	4.477%
25	12.910	1838	1840	1841	rBV	2695	2102	1.61%	0.146%
26	12.933	1841	1844	1847	rVB	123048	92744	70.84%	6.448%
27	13.016	1853	1858	1860	rBB2	1826	2683	2.05%	0.187%
28	13.115	1873	1875	1878	rVB	3597	3646	2.78%	0.253%
29	13.157	1879	1882	1884	rBV	3426	3015	2.30%	0.210%
30	13.186	1884	1887	1889	rVB	2622	2500	1.91%	0.174%
31	13.221	1890	1893	1895	rBB2	2151	2189	1.67%	0.152%
32	13.439	1927	1930	1933	rBV	18786	16432	12.55%	1.142%
33	13.598	1954	1957	1959	rBB	2181	1900	1.45%	0.132%
34	13.627	1959	1962	1964	rBB	3475	2424	1.85%	0.169%
35	13.739	1978	1981	1983	rBB	3207	2904	2.22%	0.202%
36	13.763	1983	1985	1987	rBB	3224	2557	1.95%	0.178%

LSC Area Percent Report

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Sample : M3289-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.792	1987	1990	1994	rBV2	2995	3519	2.69%	0.245%
38	13.833	1994	1997	2001	rVB2	7015	7204	5.50%	0.501%
39	13.986	2016	2023	2026	rBV2	45895	61969	47.33%	4.308%
40	14.015	2026	2028	2031	rVB	25553	19656	15.01%	1.366%
41	14.092	2039	2041	2043	rBB	4152	2660	2.03%	0.185%
42	14.374	2085	2089	2092	rBB	3057	2285	1.75%	0.159%
43	14.474	2104	2106	2108	rVB	2661	1830	1.40%	0.127%
44	15.021	2195	2199	2202	rBV	26758	34645	26.46%	2.409%
45	15.045	2202	2203	2207	rVV	12050	9845	7.52%	0.684%
46	15.080	2207	2209	2214	rVB	1591	2084	1.59%	0.145%
47	15.127	2215	2217	2222	rBB2	2706	2991	2.28%	0.208%
48	15.321	2247	2250	2257	rBB	13951	14901	11.38%	1.036%
49	15.386	2257	2261	2265	rBV	19734	21982	16.79%	1.528%
50	15.445	2267	2271	2275	rBV	29554	34574	26.41%	2.404%
51	15.474	2275	2276	2279	rVB	5482	3640	2.78%	0.253%
52	15.886	2342	2346	2349	rVB	2252	2444	1.87%	0.170%
53	16.380	2428	2430	2434	rBB	1566	1780	1.36%	0.124%
54	16.621	2466	2471	2474	rBV2	1712	2554	1.95%	0.178%
55	16.898	2512	2518	2524	rBV2	6891	12490	9.54%	0.868%
56	17.074	2543	2548	2551	rBB2	911	1758	1.34%	0.122%
57	17.339	2588	2593	2598	rBB2	5064	9565	7.31%	0.665%

Sum of corrected areas: 1438444

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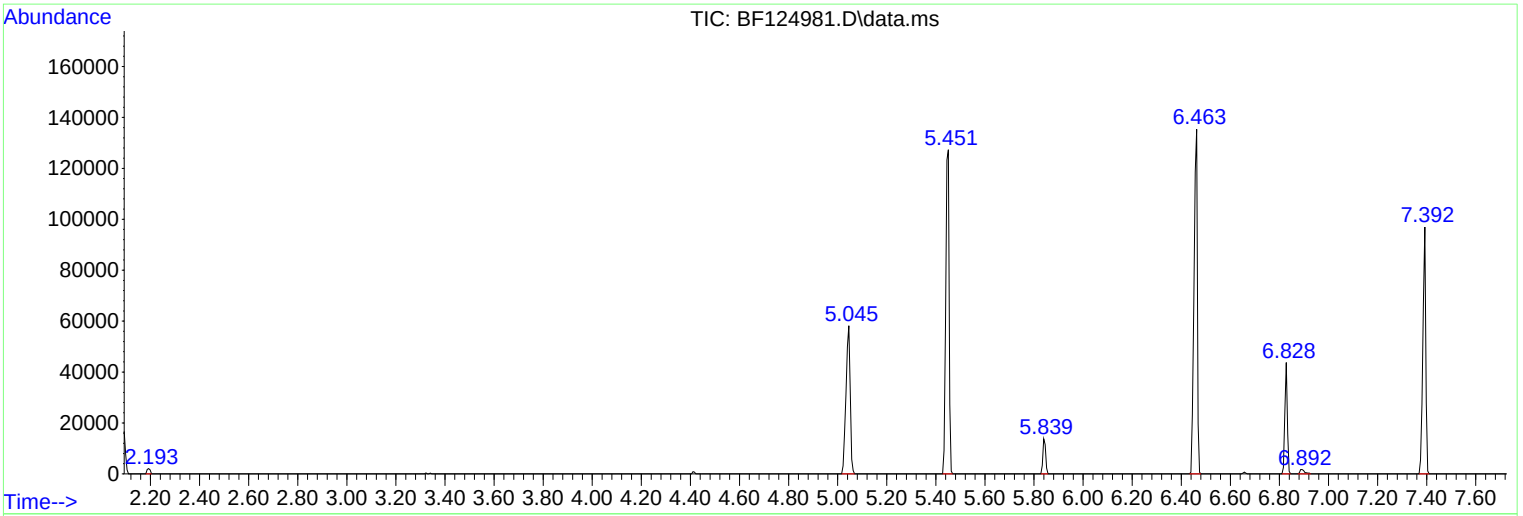
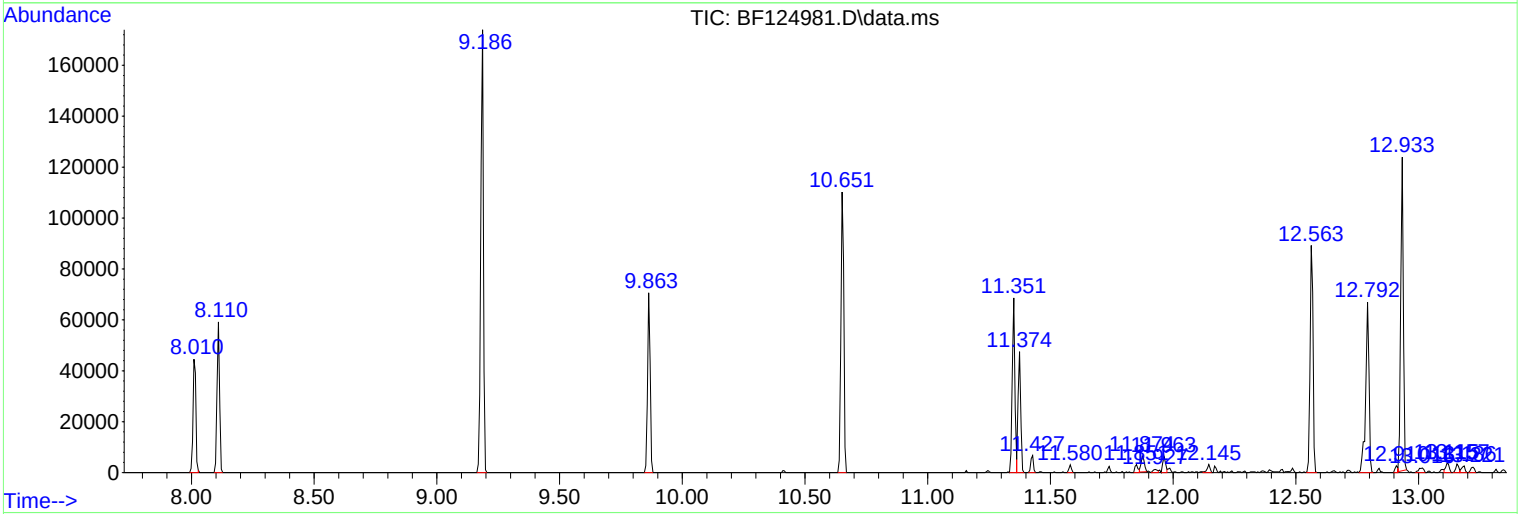
Misc :
ALS Vial : 8 Sample Multiplier: 1

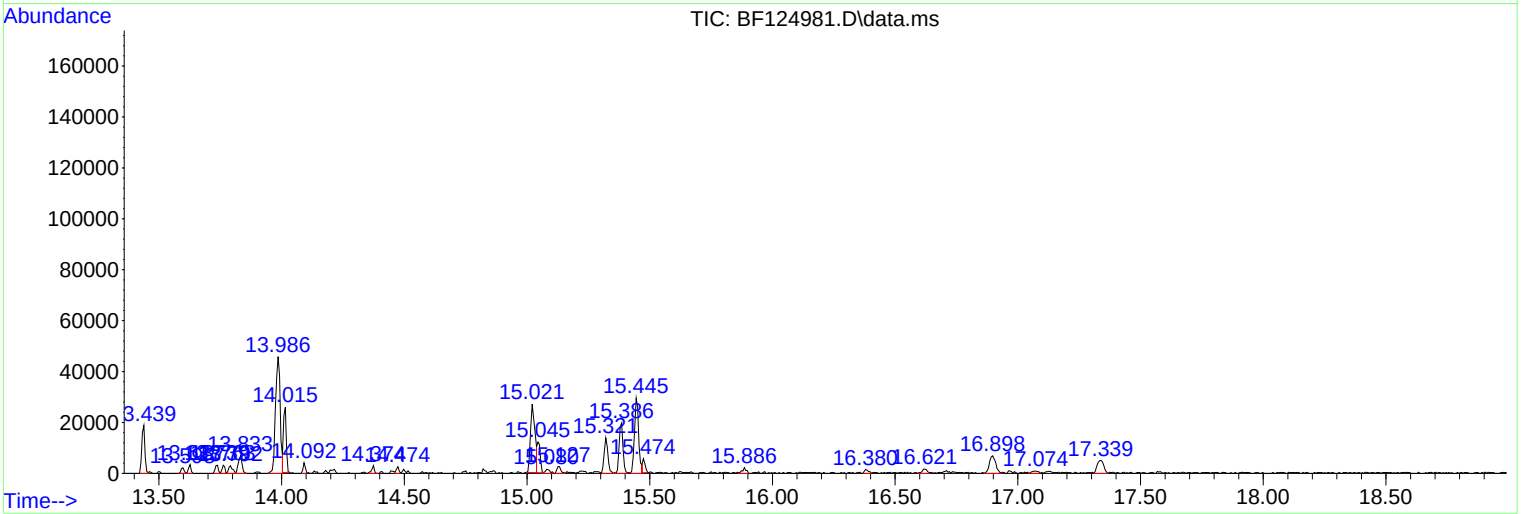
Instrument :
BNA_F
ClientSampleId :
26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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TIC Library : C:\Database\NIST20.L
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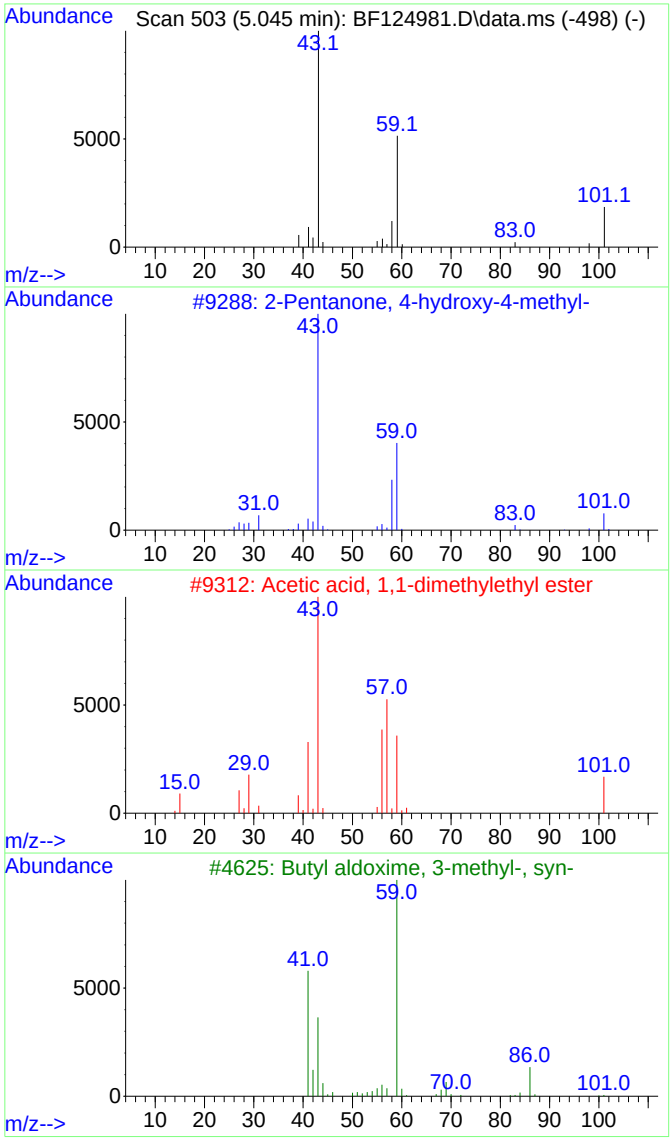
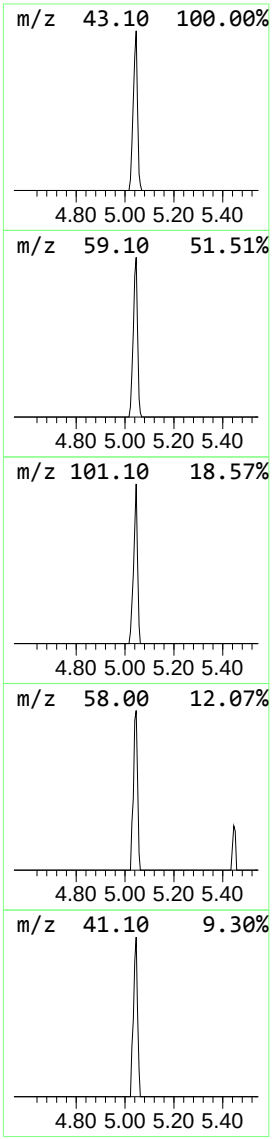
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	45.26 ng	69619	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Operator : JU/CG
Sample : M3289-11
Misc :
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Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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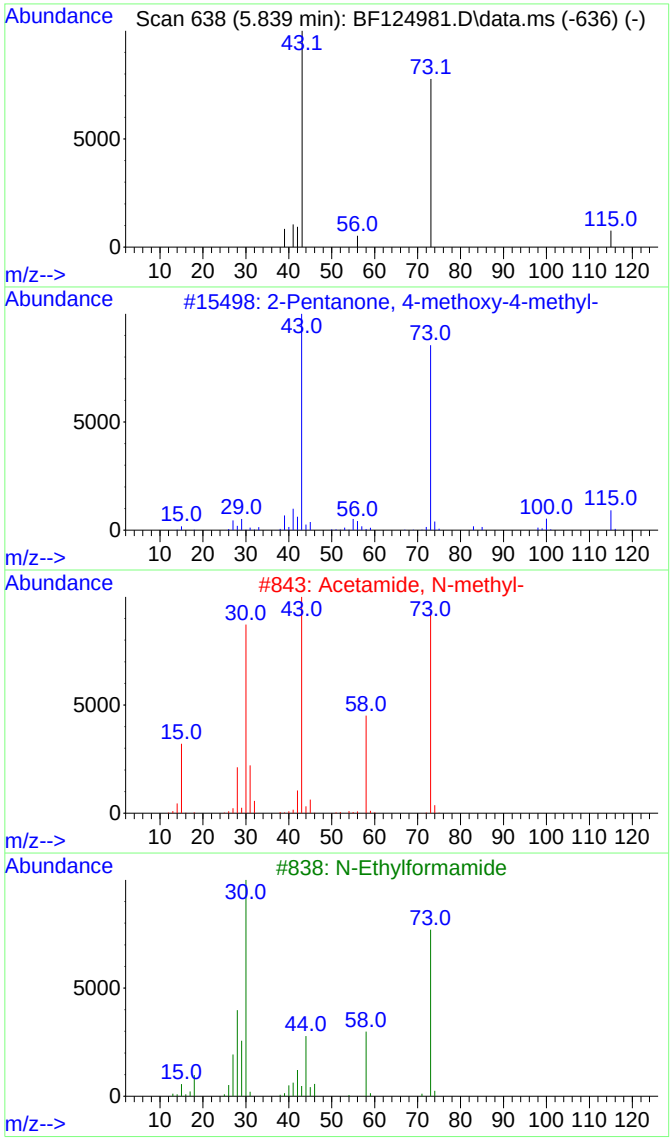
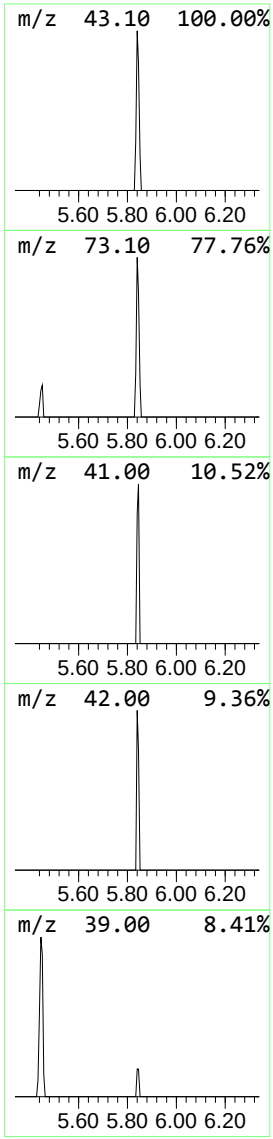
****

Peak Number 2 unknown5.839 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.839	7.10 ng	10926	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	9
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
3	N-Ethylformamide	73	C3H7NO	000627-45-2	5
4	Morpholine, 2,6-dimethyl-, cis-	115	C6H13NO	006485-55-8	4
5	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	4





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Sample : M3289-11
Misc :
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Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

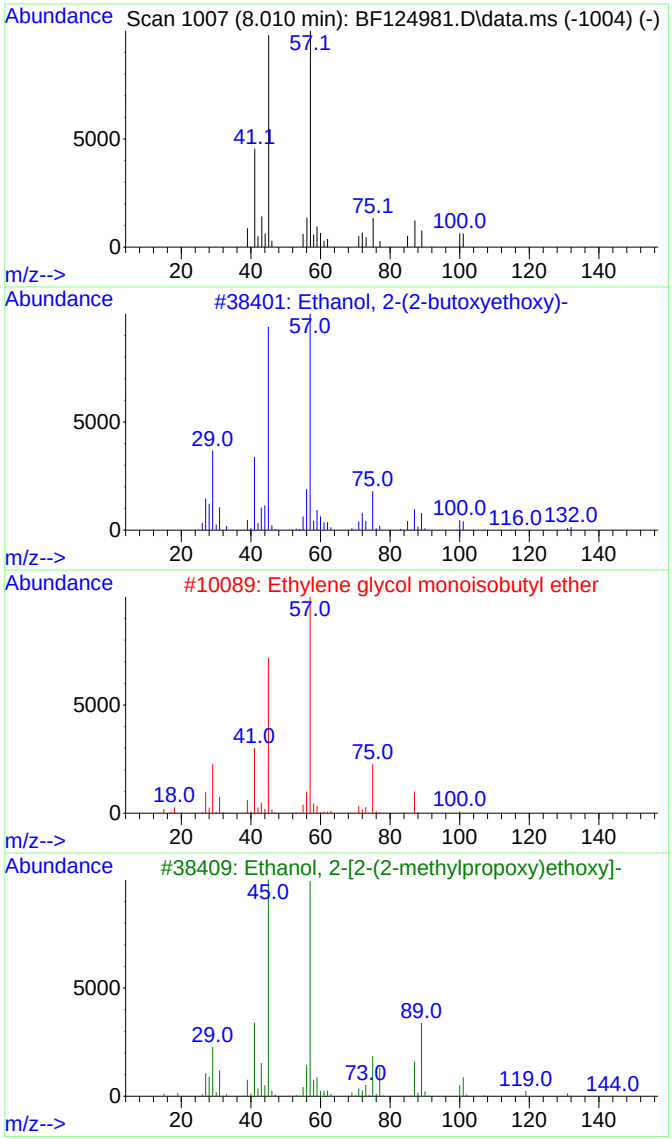
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

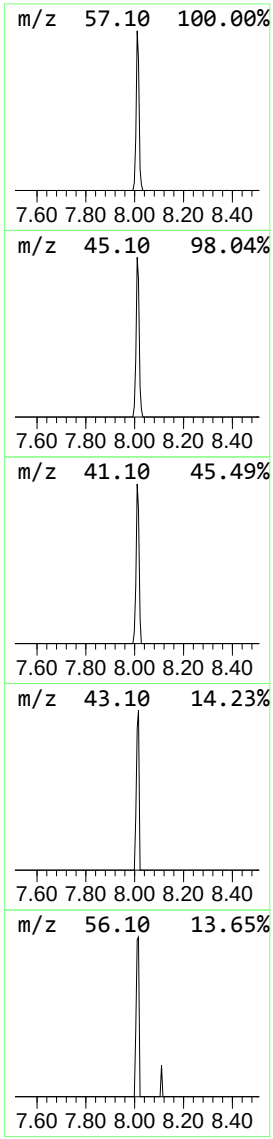
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.010	16.87 ng	36356	Naphthalene-d8	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Instrument : BNA_F
ClientSampleId : 26498

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

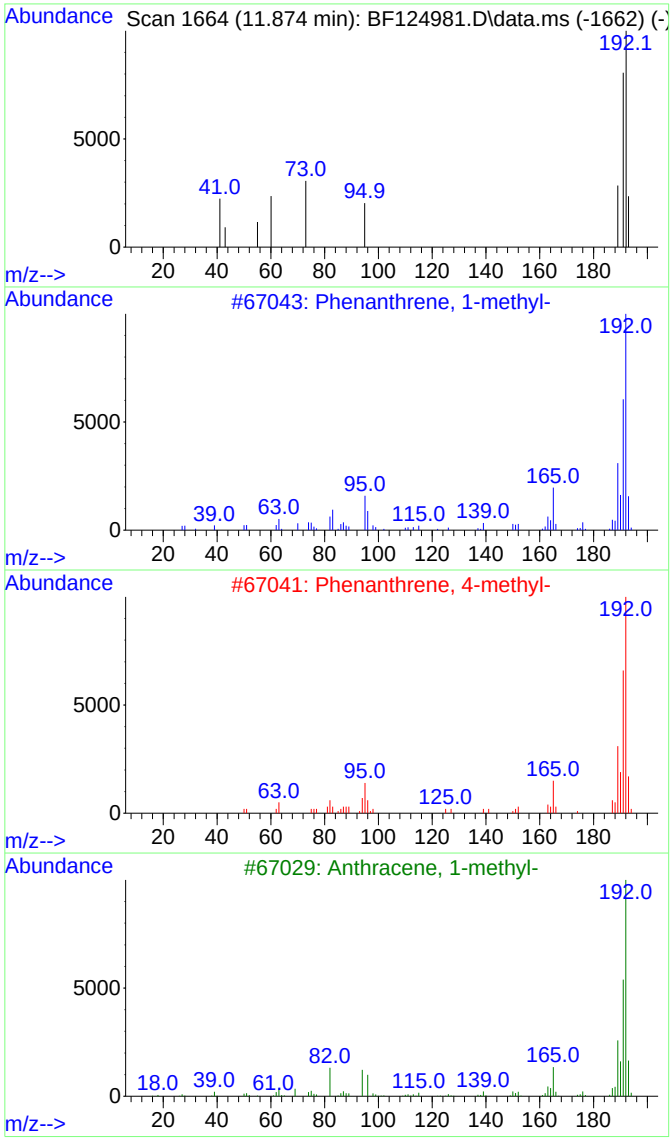
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

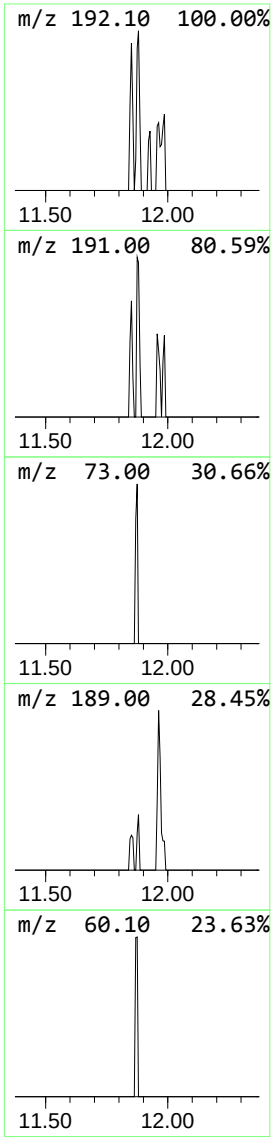
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	2.16 ng	5616	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	64
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	9
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	9
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	9





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Instrument : BNA_F
ClientSampleId : 26498

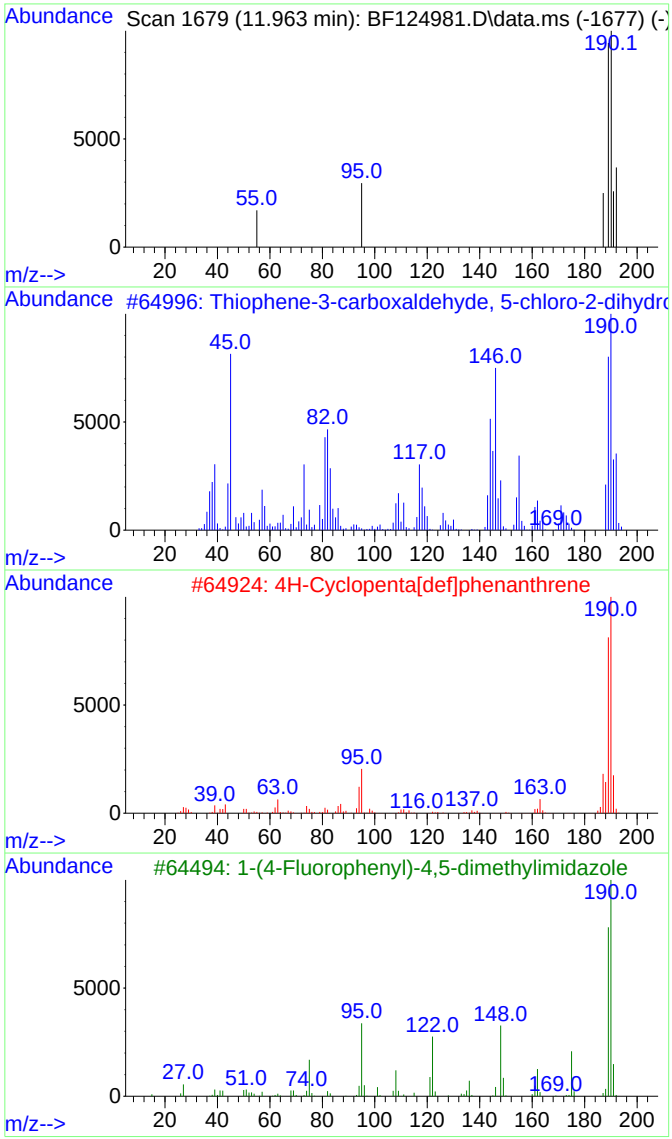
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

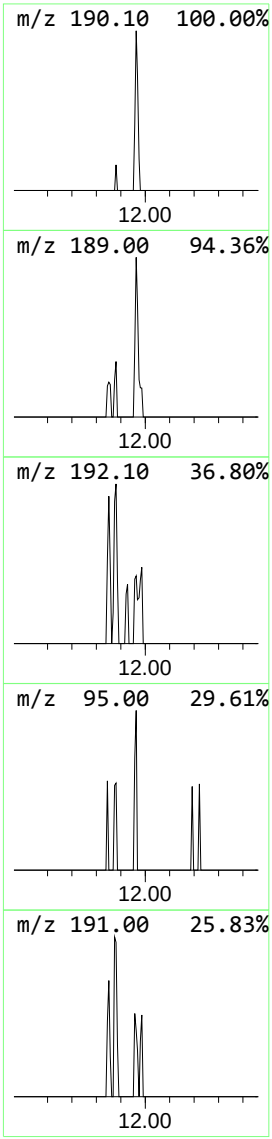
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Thiophene-3-carboxaldehyde,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	2.05 ng	5318	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	83
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	78
3	1-(4-Fluorophenyl)-4,5-dimethyli...	190	C11H11FN2	1000443-18-7	56
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	2-Chloro-1-(2-propynyl)-1H-benzi...	190	C10H7ClN2	080276-19-3	9





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TIC Library : C:\Database\NIST20.L
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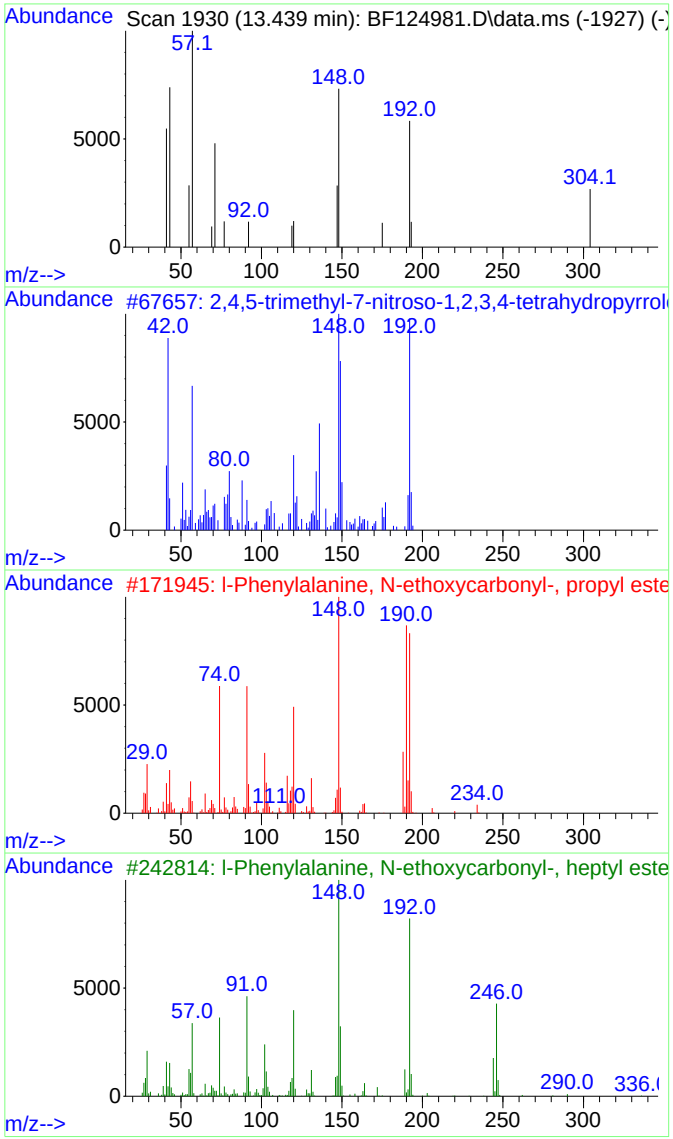
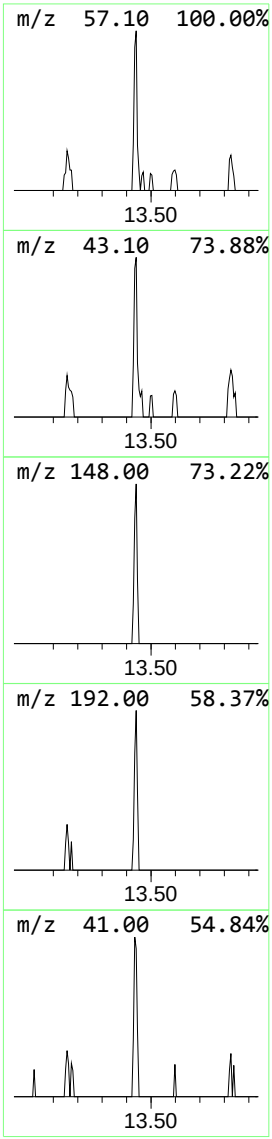
****

Peak Number 6 unknown13.439 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	5.30 ng	16432	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5-trimethyl-7-nitroso-1,2,3,...	193	C10H15N3O	1000451-78-3	43
2	l-Phenylalanine, N-ethoxycarbony...	279	C15H21NO4	1000313-72-6	28
3	l-Phenylalanine, N-ethoxycarbony...	335	C19H29NO4	1000313-73-0	28
4	2(3H)-Benzoxazolimine, 3-methyl-	148	C8H8N2O	018034-93-0	25
5	1-Methyl-1H-pyrazolo[3,4-b]pyrid...	148	C7H8N4	072583-83-6	25





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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

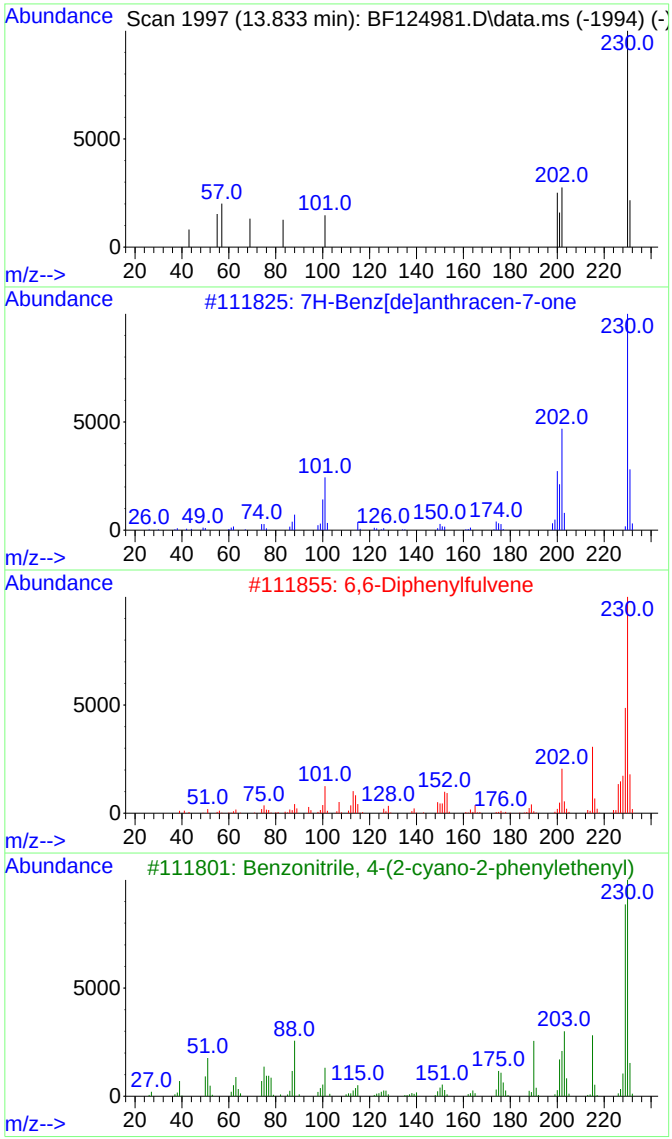
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

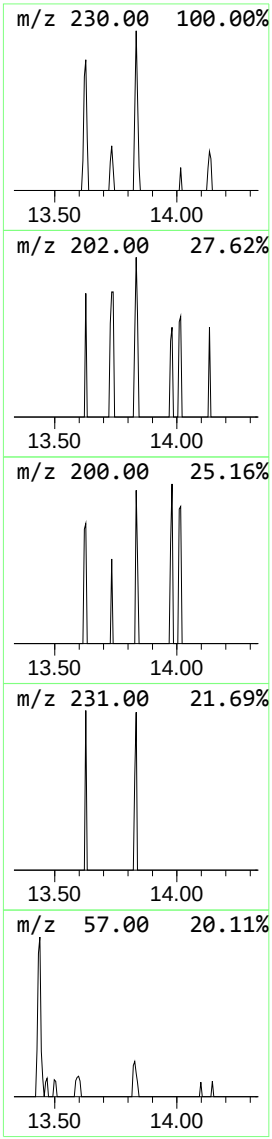
****

Peak Number 7 7H-Benz[de]anthracen-7-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	2.33 ng	7204	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	80
2	6,6-Diphenylfulvene	230	C18H14	002175-90-8	64
3	Benzonitrile, 4-(2-cyano-2-pheny...	230	C16H10N2	061469-58-7	64
4	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	64
5	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	59





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Acq On : 7 Aug 2021 18:58
Operator : JU/CG
Sample : M3289-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

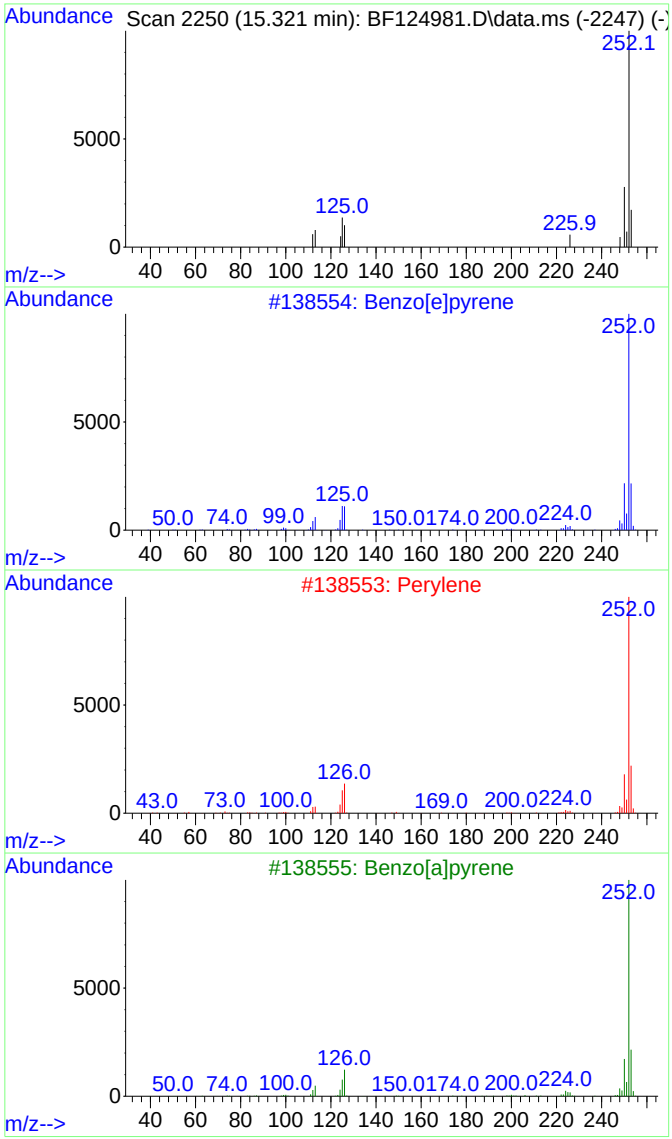
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

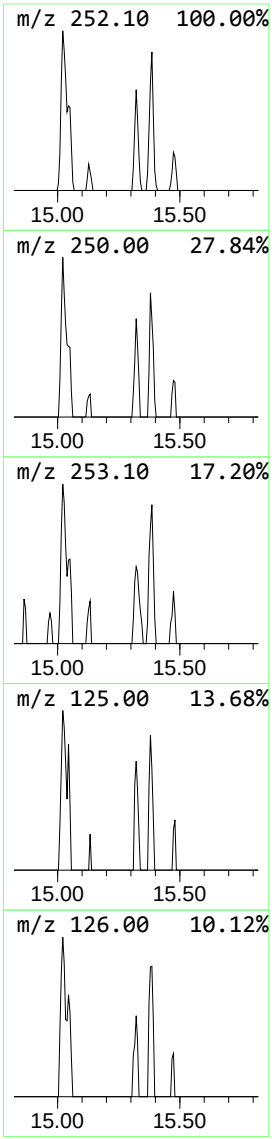
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	8.62 ng	14901	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	87
2	Perylene	252	C20H12	000198-55-0	80
3	Benzo[a]pyrene	252	C20H12	000050-32-8	80
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	80
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124981.D
Acq On : 7 Aug 2021 18:58
Operator : JU/CG
Sample : M3289-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26498

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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-...	5.045	45.3	ng	69619	1	6.828	30764	20.0
unknown5.839	5.839	7.1	ng	10926	1	6.828	30764	20.0
Ethanol, 2-(2-b...	8.010	16.9	ng	36356	2	8.110	43098	20.0
Phenanthrene, 1...	11.874	2.2	ng	5616	4	11.351	51885	20.0
Thiophene-3-car...	11.963	2.0	ng	5318	4	11.351	51885	20.0
unknown13.439	13.439	5.3	ng	16432	5	13.992	61969	20.0
7H-Benz[de]anth...	13.833	2.3	ng	7204	5	13.992	61969	20.0
Benzo[e]pyrene	15.321	8.6	ng	14901	6	15.445	34574	20.0