LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	451	455	475	rBV	630398	838091	26.12%	3.377%
2	5.387	524	527	551	rBV	2438394	2737849	85.32%	11.031%
3	5.763	588	591	599	rBV	61409	59462	1.85%	0.240%
4	6.410	698	701	717	rBV	2783688	2714828	84.61%	10.938%
5	6.745	755	758	766	rVB	918956	749253	23.35%	3.019%
6	7.322	852	856	866	rBV	1985537	1800253	56.10%	7.253%
7	8.028	973	976	980	rBV	1212744	978143	30.48%	3.941%
8	9.104	1155	1159	1162	rBV	4162544	3208765	100.00%	12.928%
9	9.375	1201	1205	1210	rBV2	55077	50184	1.56%	0.202%
10	9.780	1271	1274	1278	rBV	1299336	999495	31.15%	4.027%
11	10.574	1406	1409	1422	rBV	1688962	1561846	48.67%	6.293%
12	11.269	1524	1527	1530	rBV	953745	829815	25.86%	3.343%
13	11.292	1530	1531	1536	rVV	326020	256057	7.98%	1.032%
14	11.351	1536	1541	1546	rVV	52733	61531	1.92%	0.248%
15	11.516	1563	1569	1573	rBV2	45534	61231	1.91%	0.247%
16	11.651	1589	1592	1595	rVB	97011	77494	2.42%	0.312%
17	11.774	1610	1613	1615	rBV	67597	62167	1.94%	0.250%
18	11.804	1615	1618	1624	rVB2	89871	97616	3.04%	0.393%
19	11.886	1629	1632	1634	rVV2	83870	87507	2.73%	0.353%
20	11.910	1634	1636	1640	rVB	51893	42424	1.32%	0.171%
21	12.321	1703	1706	1708	rBV	49964	45593	1.42%	0.184%
22	12.351	1708	1711	1715	rVB3	71442	74789	2.33%	0.301%
23	12.439	1722	1726	1731	rVB2	61988	63560	1.98%	0.256%
24	12.486	1731	1734	1739	rBV	535641	455327	14.19%	1.834%
25	12.716	1767	1773	1779	rBV	442644	470859	14.67%	1.897%
26	12.851	1792	1796	1800	rBV	2334517	1928131	60.09%	7.768%
27	12.933	1806	1810	1816	rBV3	34838	62964	1.96%	0.254%
28	13.045	1827	1829	1835	rVB2	74271	87919	2.74%	0.354%
29	13.151	1843	1847	1854	rVB3	54609	83053	2.59%	0.335%
30	13.245	1859	1863	1866	rBV	40106	41230	1.28%	0.166%
31	13.568	1915	1918	1925	rVB	44596	45217	1.41%	0.182%
32	13.674	1930	1936	1937	rBV2	58367	67569	2.11%	0.272%
33	13.780	1951	1954	1959	rBV	58345	86207	2.69%	0.347%
34	13.915	1971	1977	1980	rBV2	721037	919889	28.67%	3.706%
35	13.945	1980	1982	1989	rVB	298498	261152	8.14%	1.052%
36	14.004	1989	1992	1994	rBV	103060	94525	2.95%	0.381%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.310	2039	2044	2047	rBV2	71377	81695	2.55%	0.329%
38	14.345	2047	2050	2054	rBV3	31063	45243	1.41%	0.182%
39	14.645	2097	2101	2107	rBV	615716	670884	20.91%	2.703%
40	14.804	2124	2128	2131	rBV3	30687	46914	1.46%	0.189%
41	14.951	2149	2153	2156	rBV	282209	392098	12.22%	1.580%
42	15.057	2169	2171	2175	rBV	40071	42623	1.33%	0.172%
43	15.245	2199	2203	2210	rVB	160903	184832	5.76%	0.745%
44	15.309	2210	2214	2220	rBV	202599	272162	8.48%	1.097%
45	15.362	2220	2223	2228	rBV	514466	630148	19.64%	2.539%
46	15.592	2256	2262	2268	rVB5	21735	48153	1.50%	0.194%
47	16.662	2440	2444	2449	rVB4	32184	51896	1.62%	0.209%
48	16.809	2465	2469	2477	rVB2	87770	166024	5.17%	0.669%
49	17.251	2540	2544	2553	rVB2	64151	125572	3.91%	0.506%

Sum of corrected areas: 24820239

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
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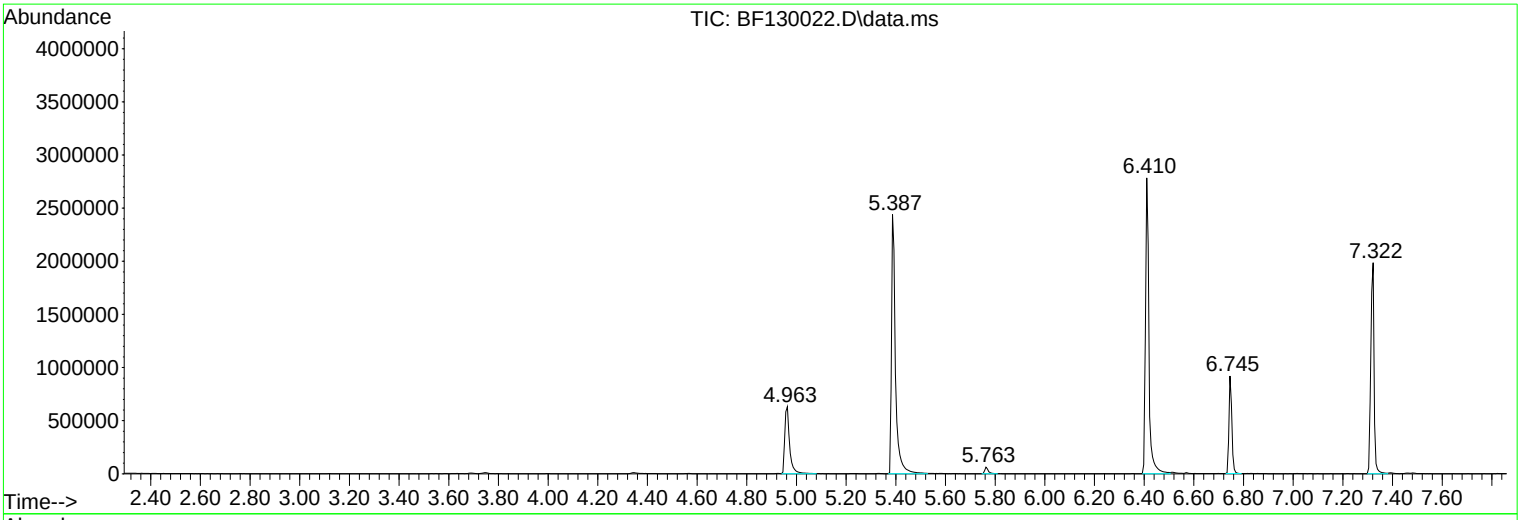
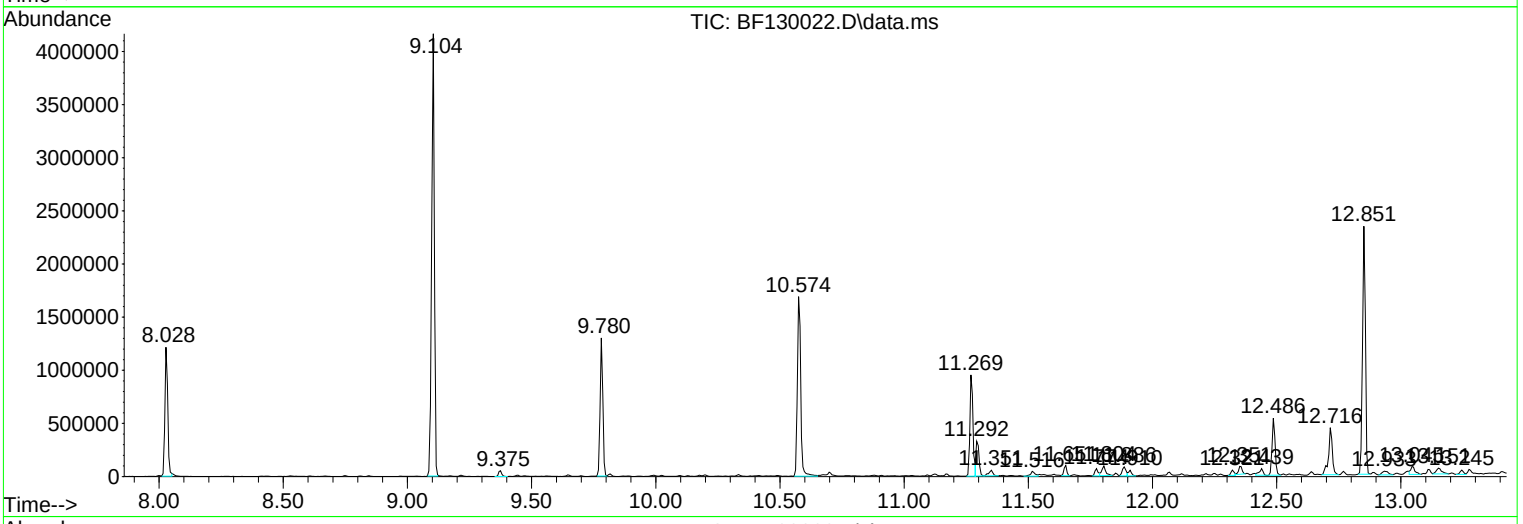
Misc :
ALS Vial : 11 Sample Multiplier: 1

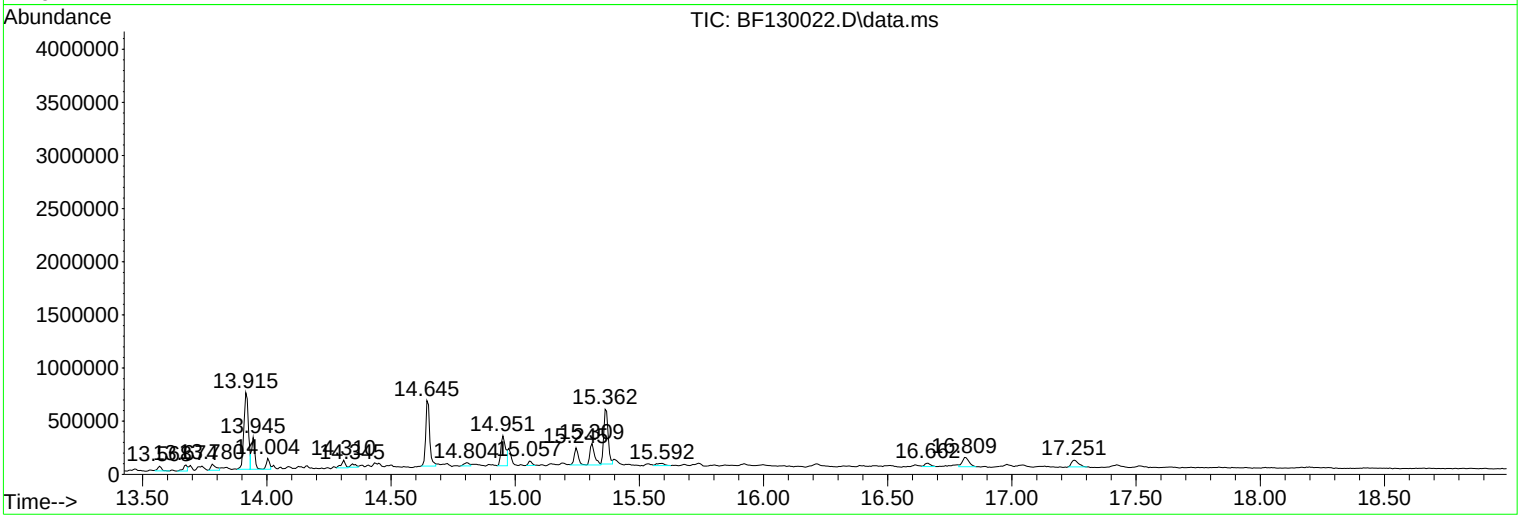
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

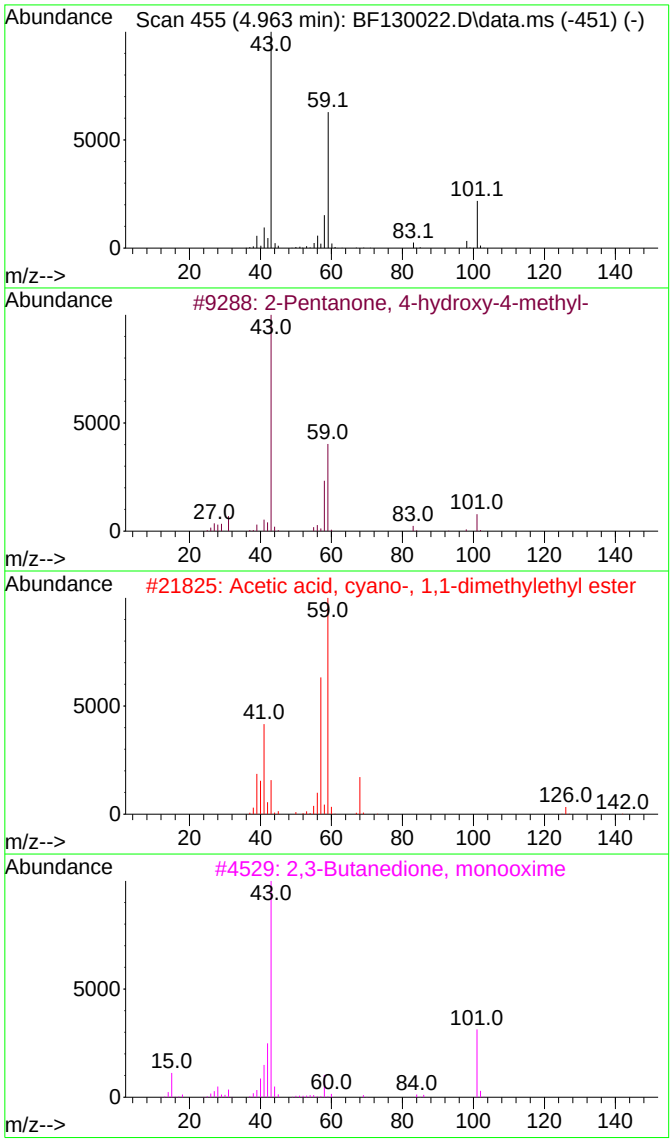
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

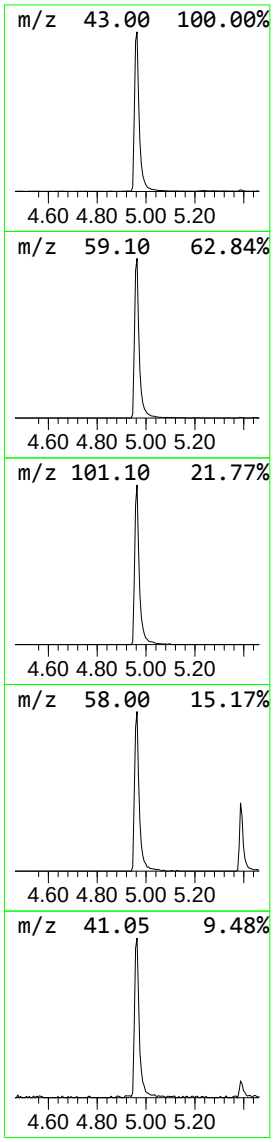
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	22.37 ng	838091	1,4-Dichlorobenzene-d4	6.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

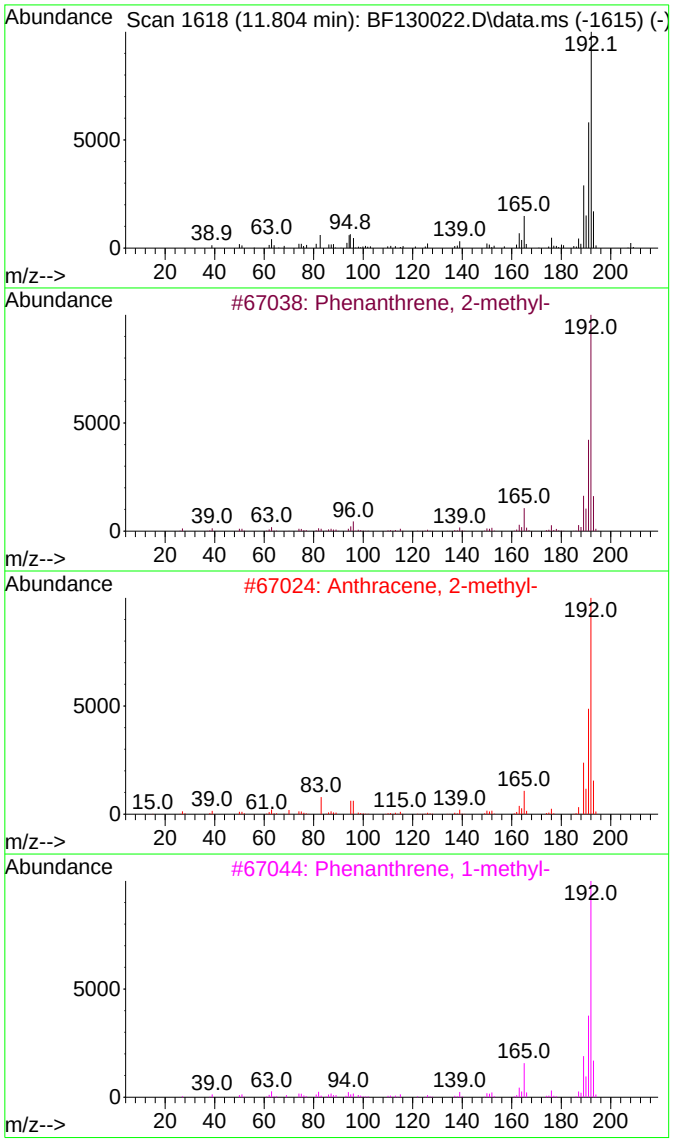
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

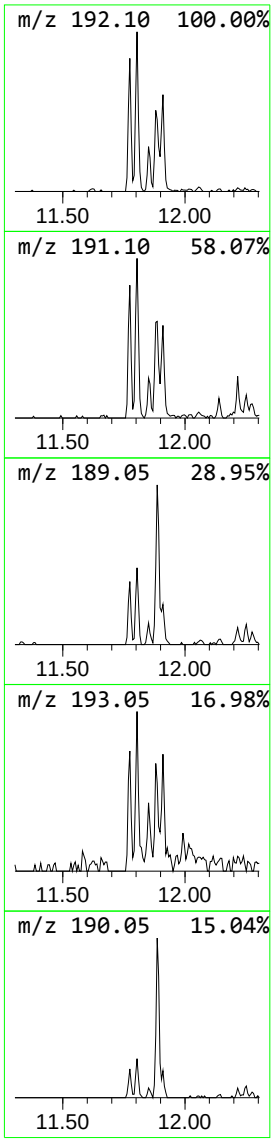
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.35 ng	97616	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

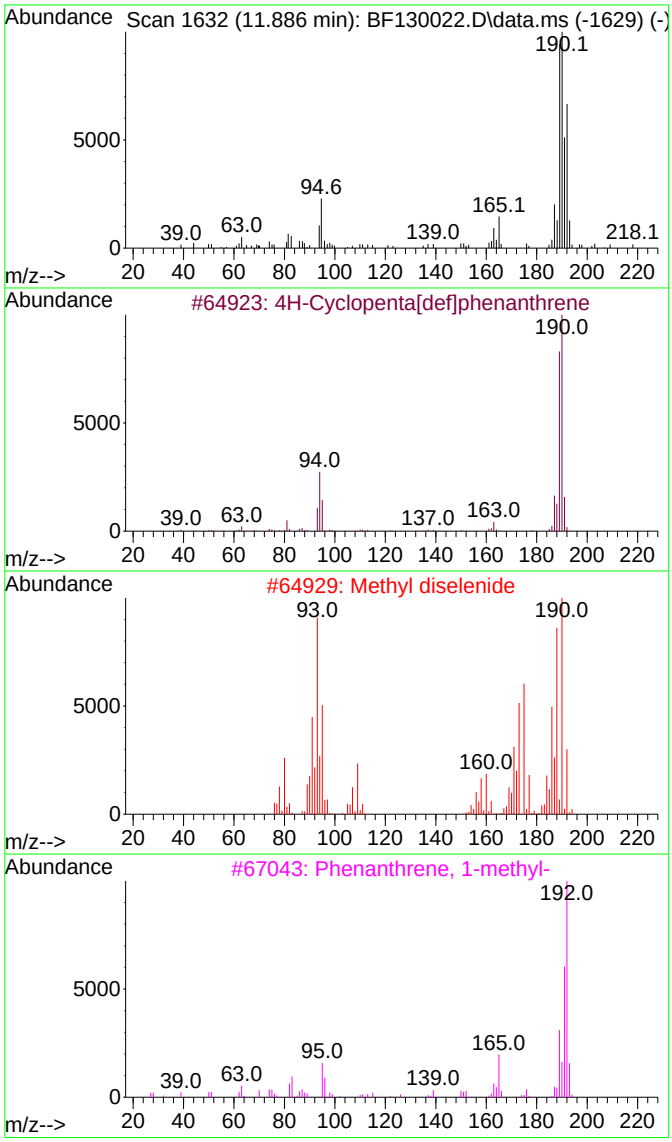
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

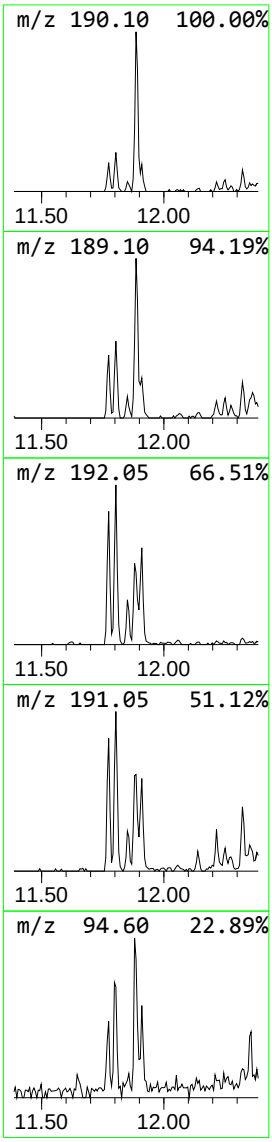
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.11 ng	87507	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

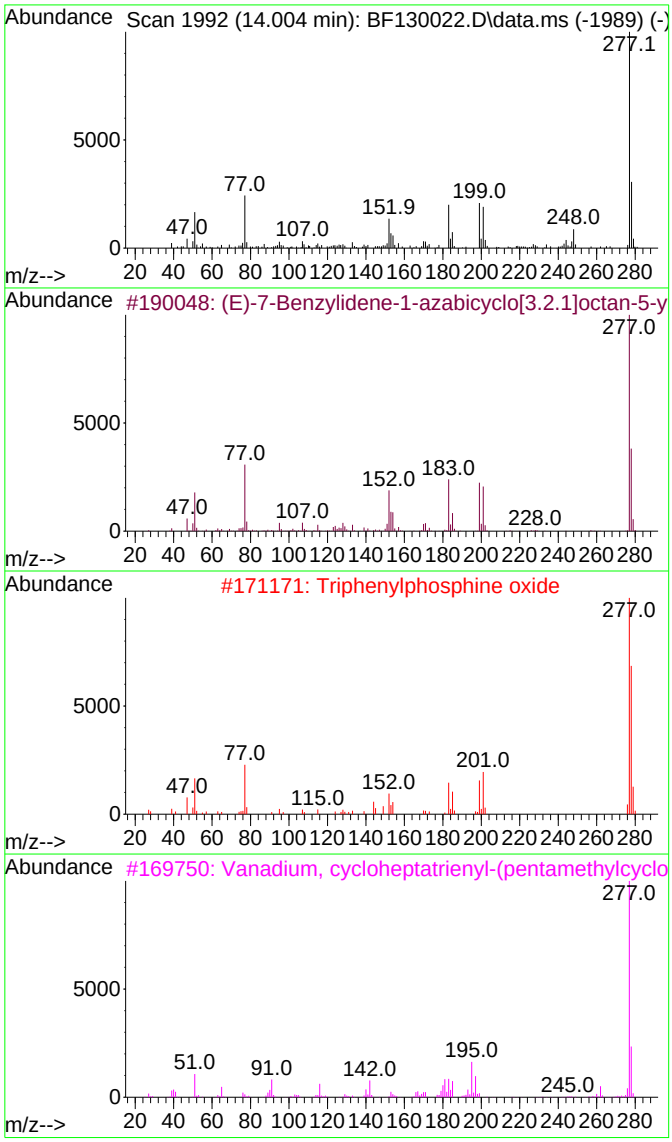
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

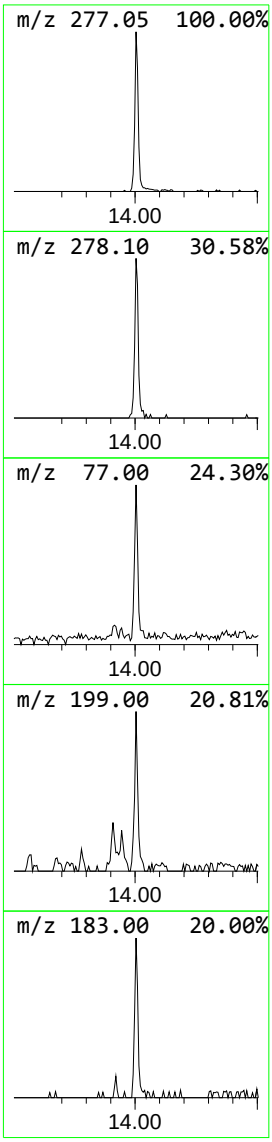
****

Peak Number 4 (E)-7-Benzylidene-1-azabicy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.06 ng	94525	Chrysene-d12	13.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	64
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
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Sample : N4375-01
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

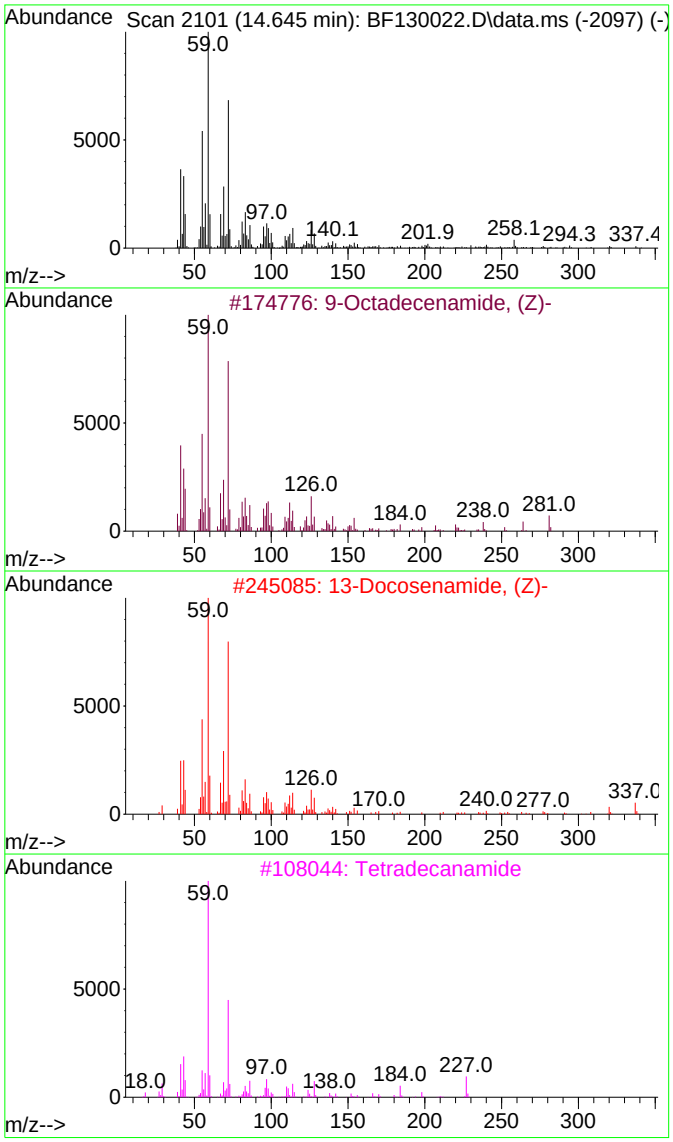
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

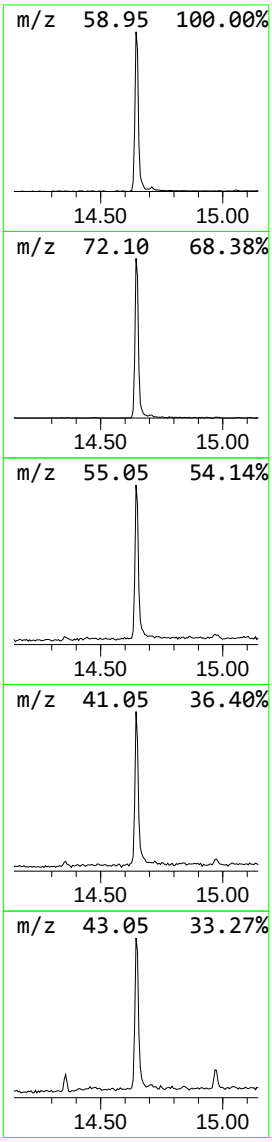
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	21.29 ng	670884	Perylene-d12	15.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Octadecanamide	283	C18H37NO	000124-26-5	50
5	O-Methyl-L-threonine, N-(methoxy...	205	C8H15NO5	1000453-27-0	38





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

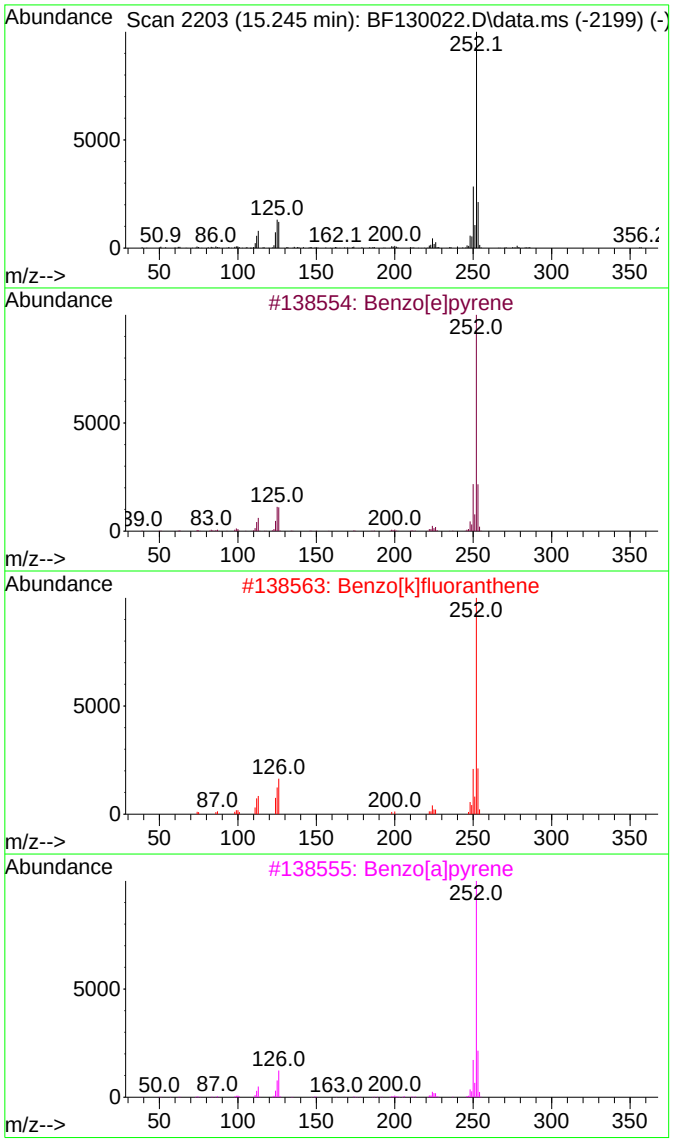
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

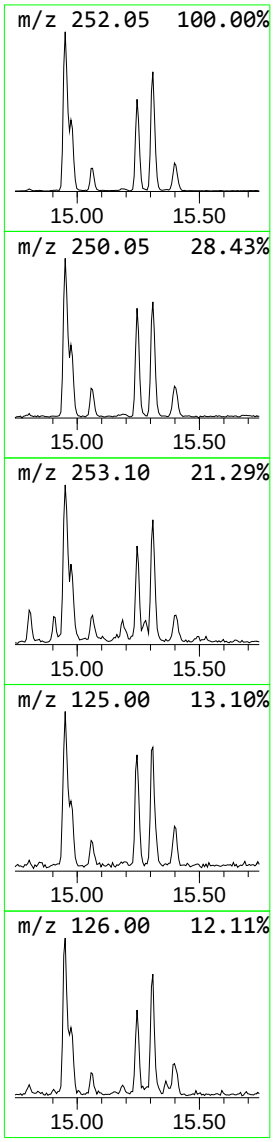
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	5.87 ng	184832	Perylene-d12	15.368

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	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130022.D
Acq On : 26 Aug 2022 16:48
Operator : CG\JU
Sample : N4375-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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-...	4.963	22.4	ng	838091	1	6.745	749253	20.0
Phenanthrene, 2...	11.804	2.4	ng	97616	4	11.269	829815	20.0
4H-Cyclopenta[d...	11.886	2.1	ng	87507	4	11.269	829815	20.0
(E)-7-Benzylide...	14.004	2.1	ng	94525	5	13.921	919889	20.0
9-Octadecenamid...	14.645	21.3	ng	670884	6	15.368	630148	20.0
Benzo[e]pyrene	15.245	5.9	ng	184832	6	15.368	630148	20.0