LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

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_M\Methods\8270-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	293	300	311	rBV	2061742	2958671	25.78%	3.284%
2	5.516	373	379	387	rBV	4891441	7301117	63.63%	8.103%
3	5.934	444	450	460	rBV2	110012	270660	2.36%	0.300%
4	7.128	643	653	669	rBV	4678097	7591082	66.15%	8.425%
5	7.610	731	735	745	rVB3	101781	194604	1.70%	0.216%
6	7.957	784	794	803	rBV	954224	1522451	13.27%	1.690%
7	8.498	880	886	899	rBV	83934	174709	1.52%	0.194%
8	9.128	986	993	1000	rBV	2933180	4801449	41.84%	5.329%
9	10.775	1262	1273	1278	rBV	1193174	2132525	18.58%	2.367%
10	10.822	1278	1281	1290	rVB	280713	442391	3.86%	0.491%
11	12.427	1547	1554	1562	rVB	74852	131668	1.15%	0.146%
12	13.227	1683	1690	1701	rVB	7018363	10065181	87.71%	11.171%
13	14.321	1869	1876	1882	rBV2	128506	247839	2.16%	0.275%
14	14.598	1916	1923	1930	rBV	1664846	2471860	21.54%	2.743%
15	14.663	1930	1934	1942	rVB	95356	140161	1.22%	0.156%
16	14.998	1987	1991	1999	rVB	111074	166418	1.45%	0.185%
17	15.645	2096	2101	2110	rBV2	146498	222969	1.94%	0.247%
18	15.957	2147	2154	2160	rBV	491416	700115	6.10%	0.777%
19	16.086	2170	2176	2199	rVB	4583154	7035188	61.31%	7.808%
20	17.162	2354	2359	2366	rVB2	104533	190299	1.66%	0.211%
21	17.345	2384	2390	2394	rBV	1889105	2667208	23.24%	2.960%
22	17.386	2394	2397	2403	rVB	1509579	2033640	17.72%	2.257%
23	17.480	2408	2413	2418	rVB	339108	499620	4.35%	0.554%
24	17.751	2455	2459	2470	rVB	121275	181500	1.58%	0.201%
25	18.239	2535	2542	2546	rBV2	733781	1469214	12.80%	1.631%
26	18.421	2567	2573	2576	rBV3	235393	415605	3.62%	0.461%
27	18.721	2620	2624	2628	rVB	122924	159715	1.39%	0.177%
28	18.768	2628	2632	2638	rVB3	96512	143389	1.25%	0.159%
29	19.280	2715	2719	2728	rBV3	93412	171222	1.49%	0.190%
30	19.403	2734	2740	2745	rBV	2266325	2962459	25.82%	3.288%
31	19.515	2754	2759	2763	rBV2	420936	756043	6.59%	0.839%
32	19.733	2792	2796	2797	rBV	307049	366341	3.19%	0.407%
33	19.762	2797	2801	2810	rVB	1969502	2765798	24.10%	3.070%
34	19.968	2830	2836	2841	rBV	9319539	11475124	100.00%	12.735%
35	20.256	2882	2885	2892	rVB3	255651	423305	3.69%	0.470%
36	20.356	2899	2902	2906	rBV	167418	196369	1.71%	0.218%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

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_M\Methods\8270-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.227	3047	3050	3059	rVB3	574724	891304	7.77%	0.989%
38	21.521	3094	3100	3104	rBV2	2438605	4587421	39.98%	5.091%
39	21.562	3104	3107	3116	rVB	1009741	1351948	11.78%	1.500%
40	23.215	3383	3388	3393	rBV	927226	2087565	18.19%	2.317%
41	23.744	3474	3478	3487	rVB	576766	1157387	10.09%	1.284%
42	23.844	3491	3495	3503	rVB	874970	1657425	14.44%	1.839%
43	23.962	3509	3515	3520	rBV2	1567381	2923347	25.48%	3.244%

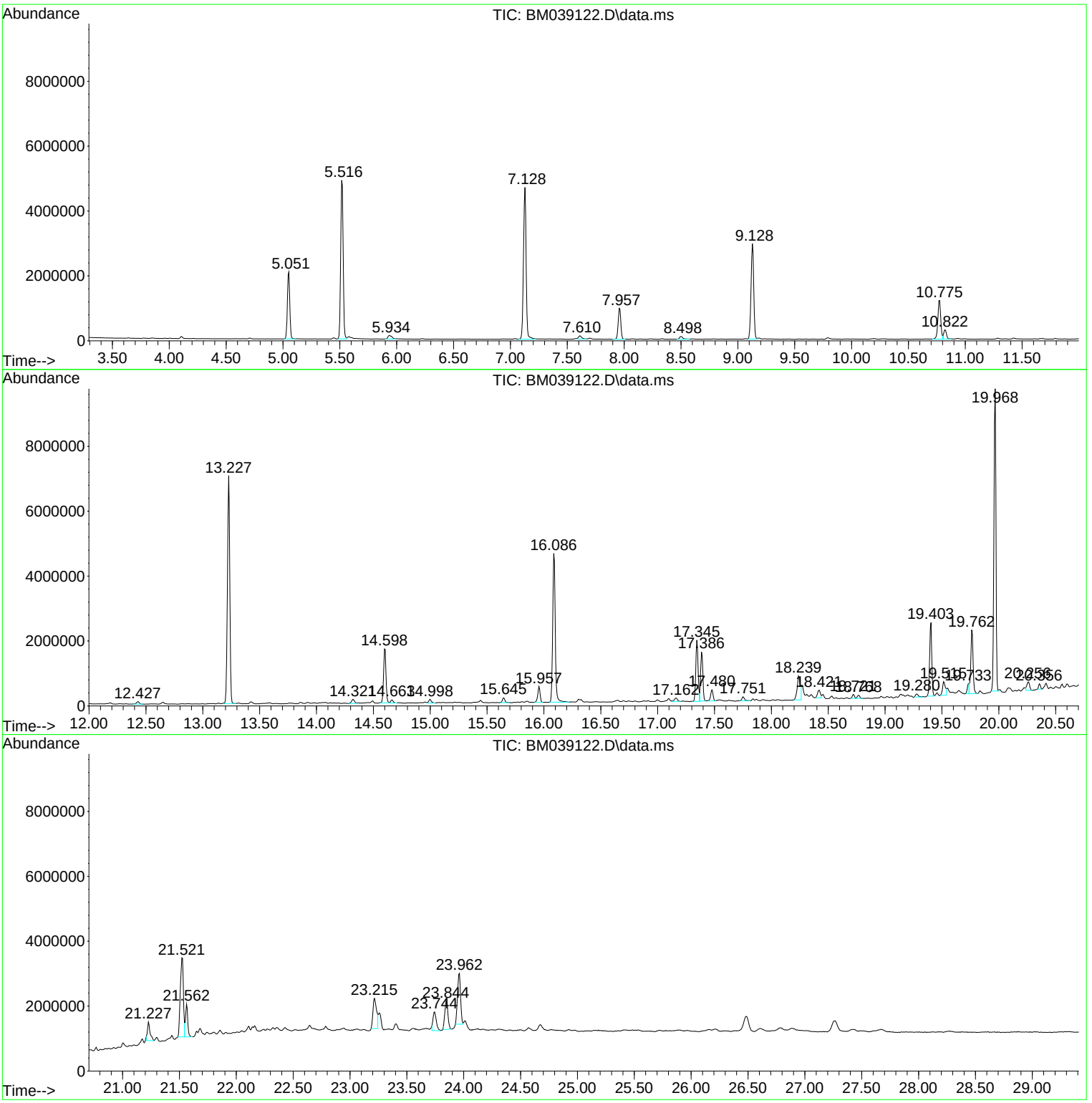
Sum of corrected areas: 90104306

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

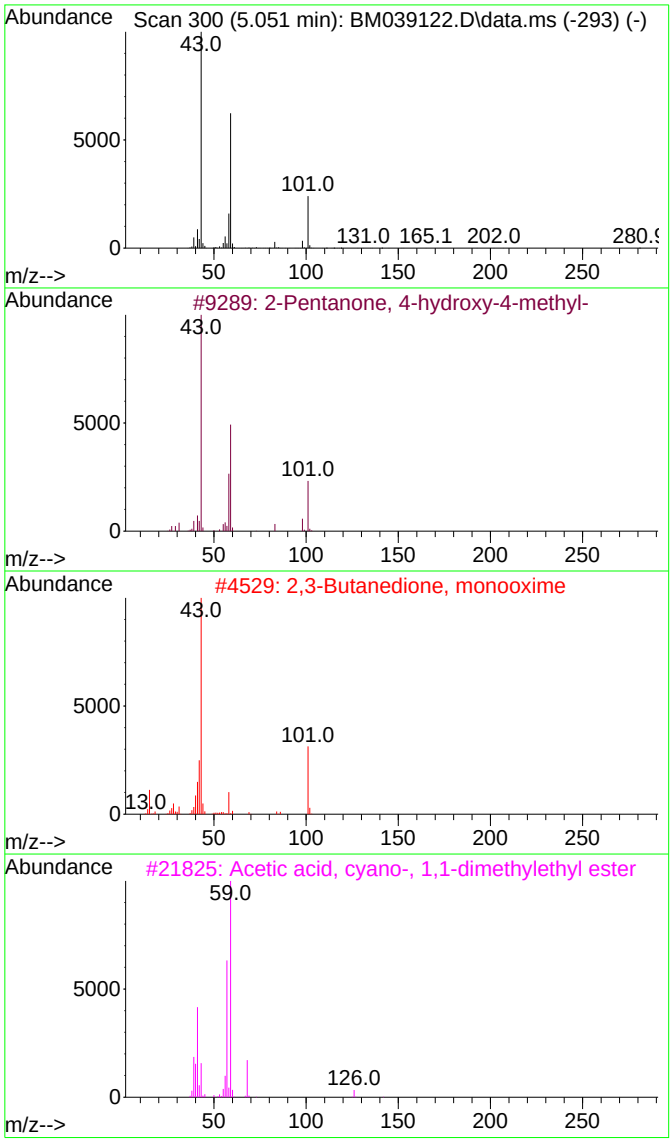
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

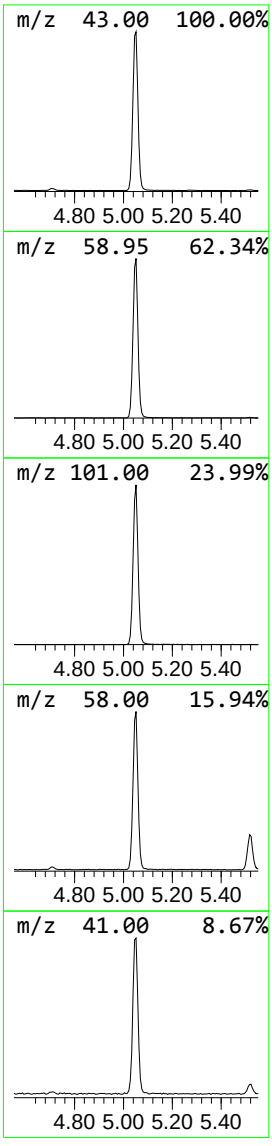
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	38.87 ng	2958670	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

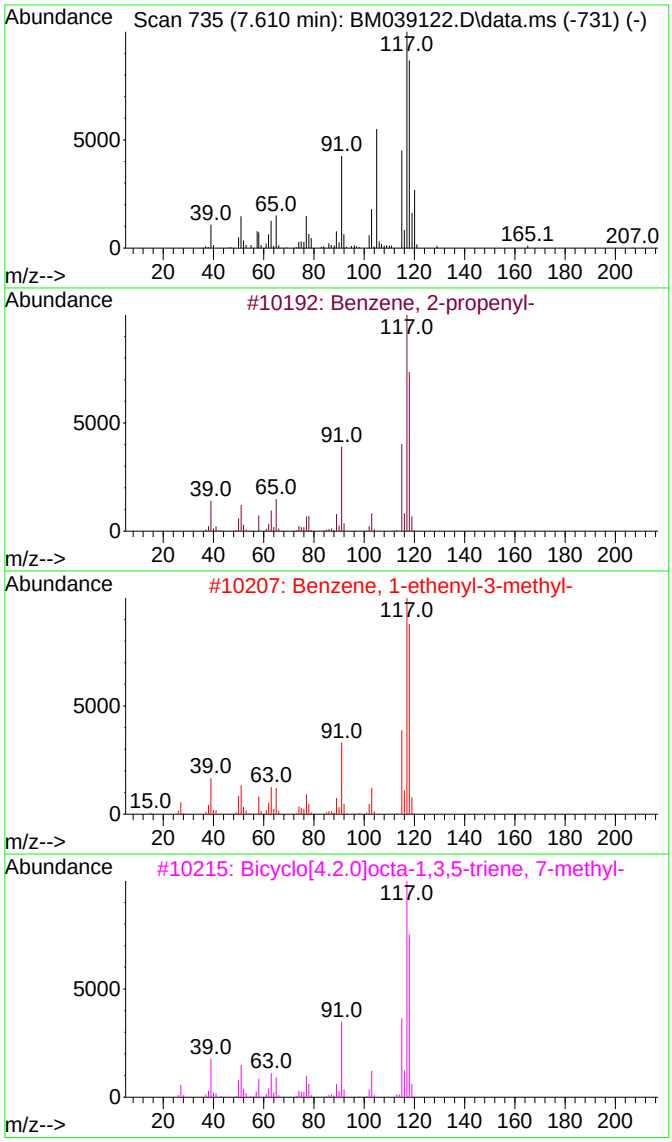
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

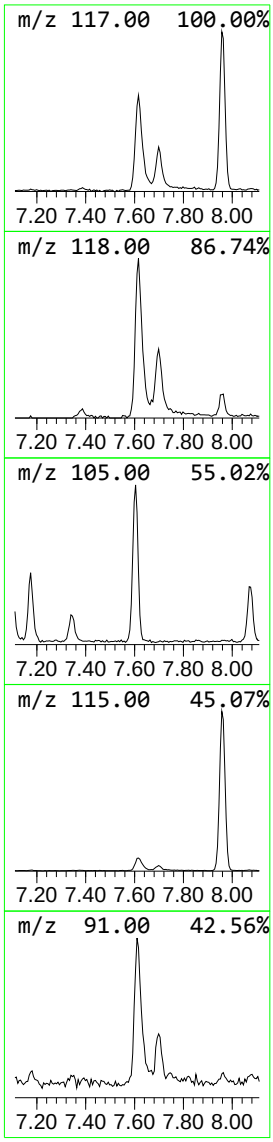
****

Peak Number 3 Benzene, 2-propenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.610	2.56 ng	194604	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	91
2	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	86
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	70
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	70
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

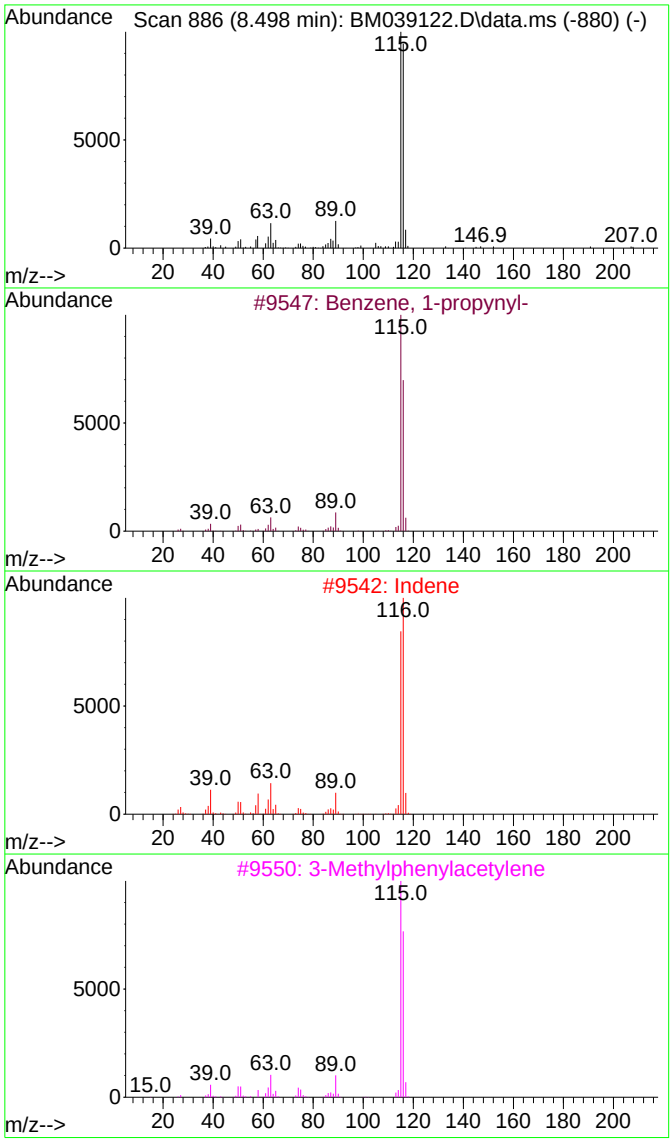
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

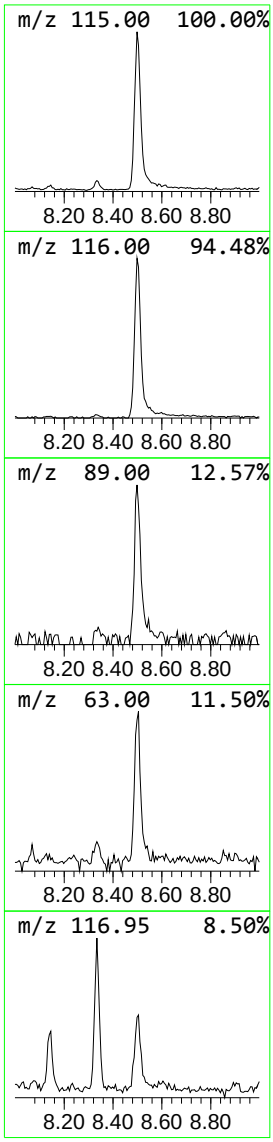
****

Peak Number 4 Benzene, 1-propynyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	2.30 ng	174709	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
2	Indene	116	C9H8	000095-13-6	93
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

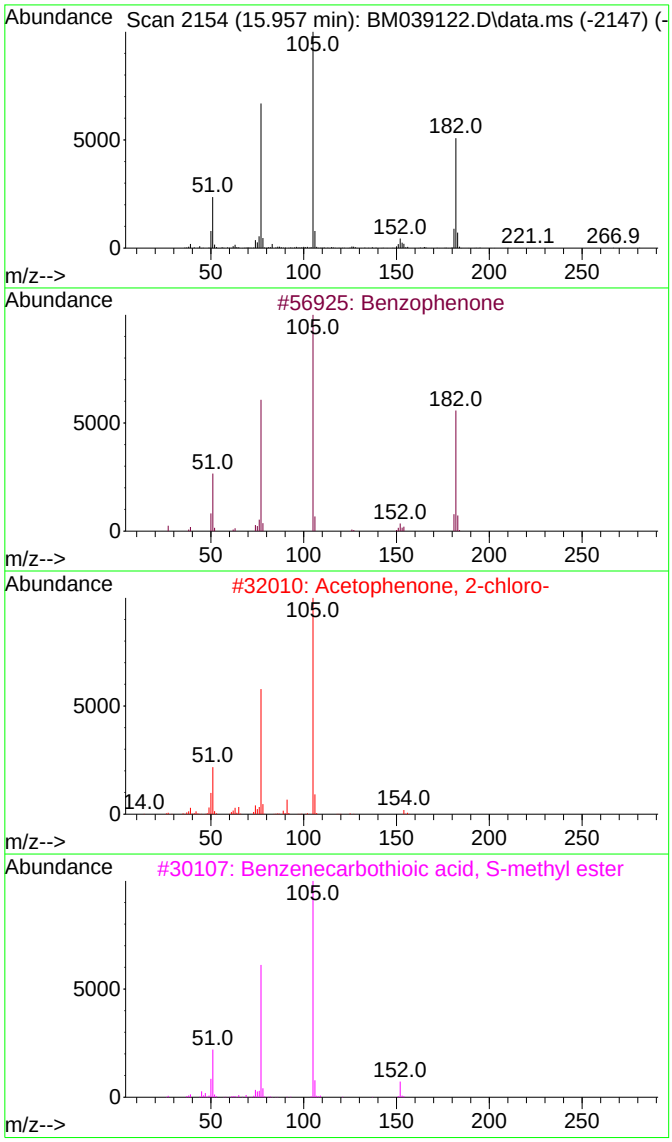
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

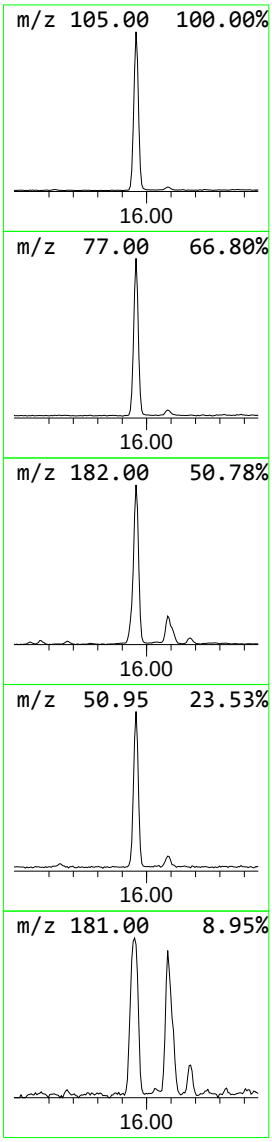
****

Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	5.66 ng	700115	Acenaphthene-d10	14.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	53
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4	Vinyl benzoate	148	C9H8O2	000769-78-8	49
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

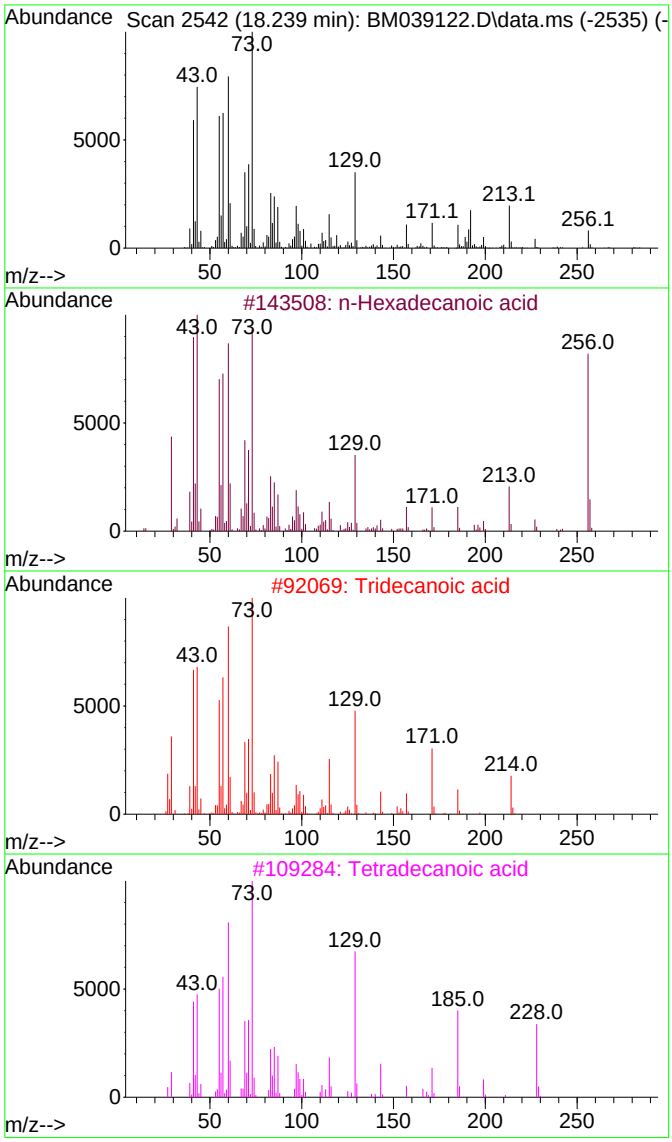
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

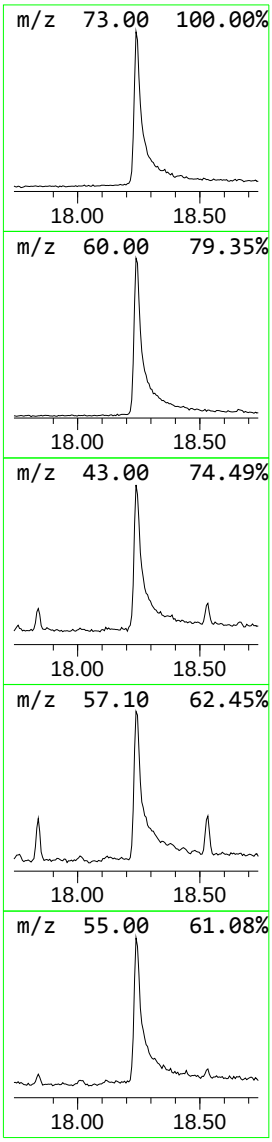
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	11.02 ng	1469210	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

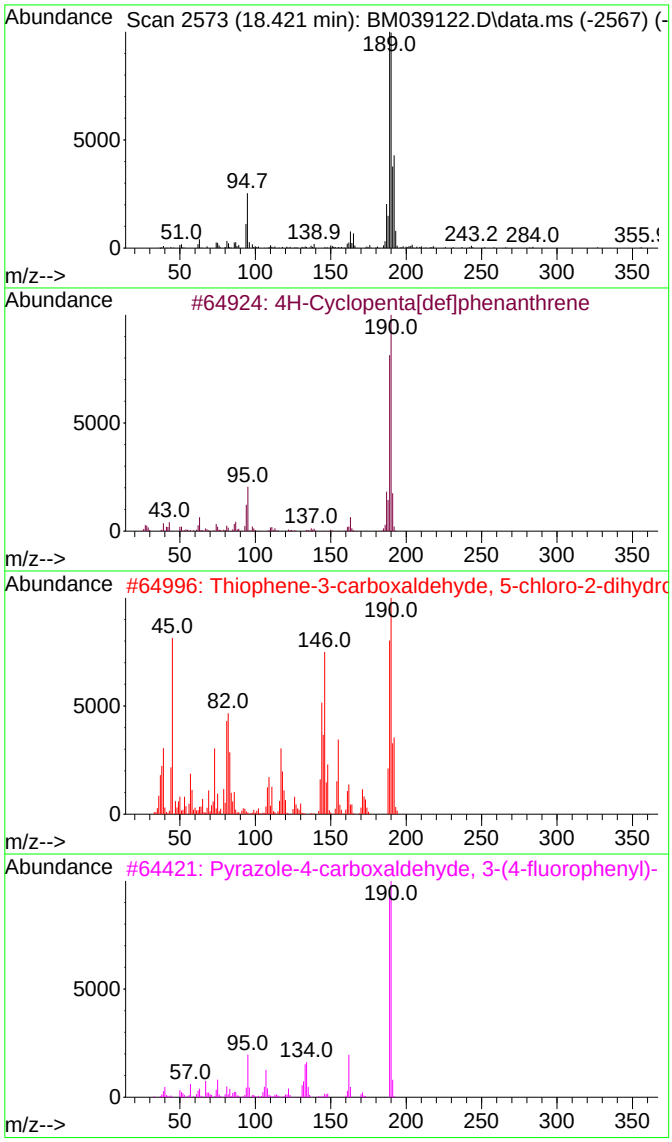
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

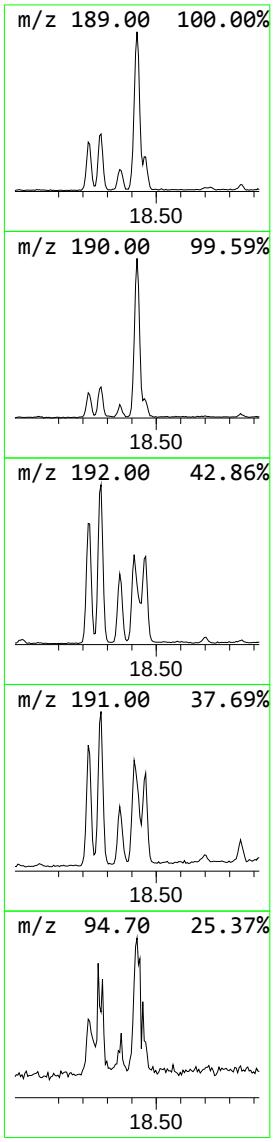
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.421	3.12 ng	415605	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	86
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

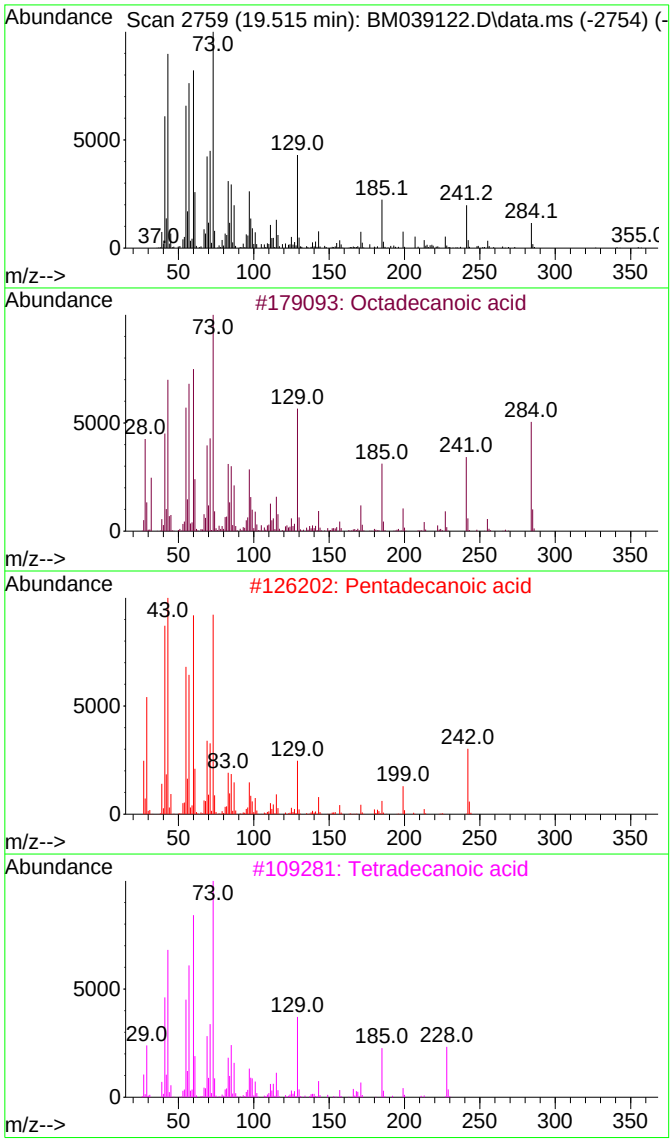
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

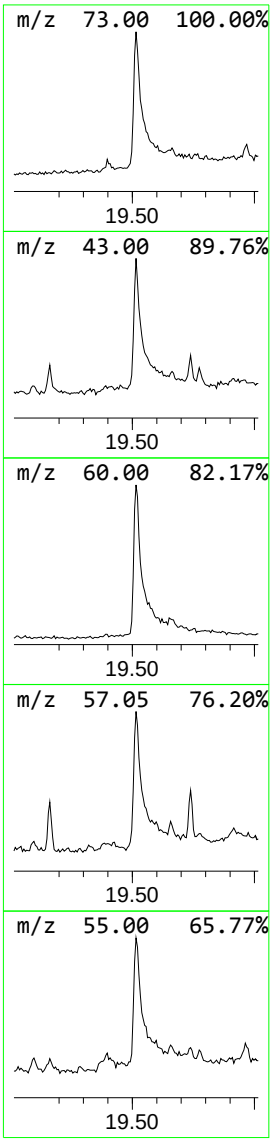
****

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	3.30 ng	756043	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

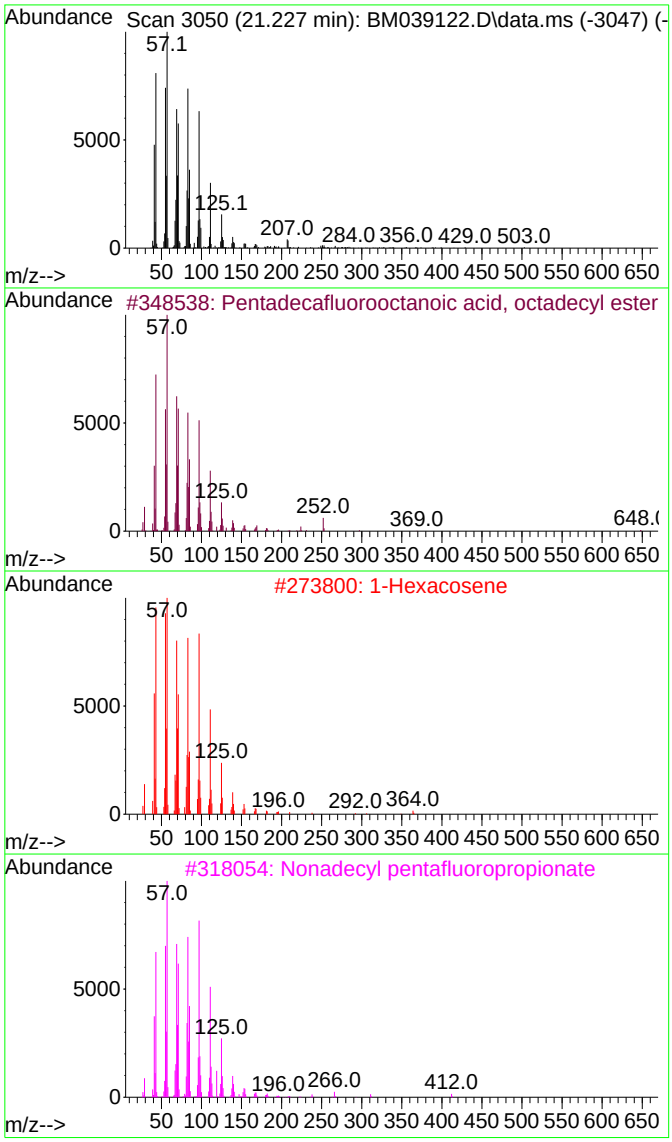
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

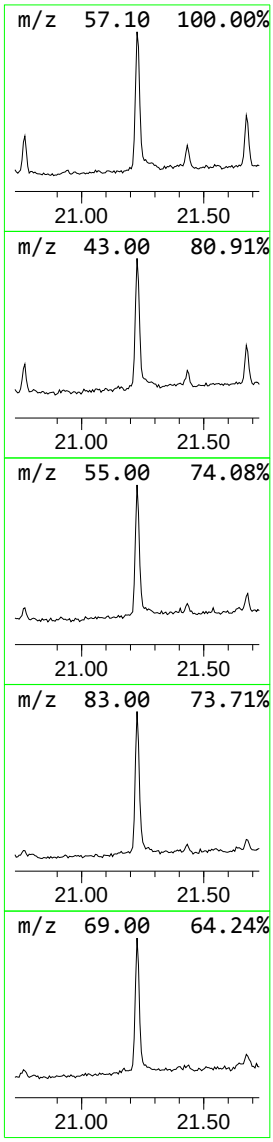
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	3.89 ng	891304	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

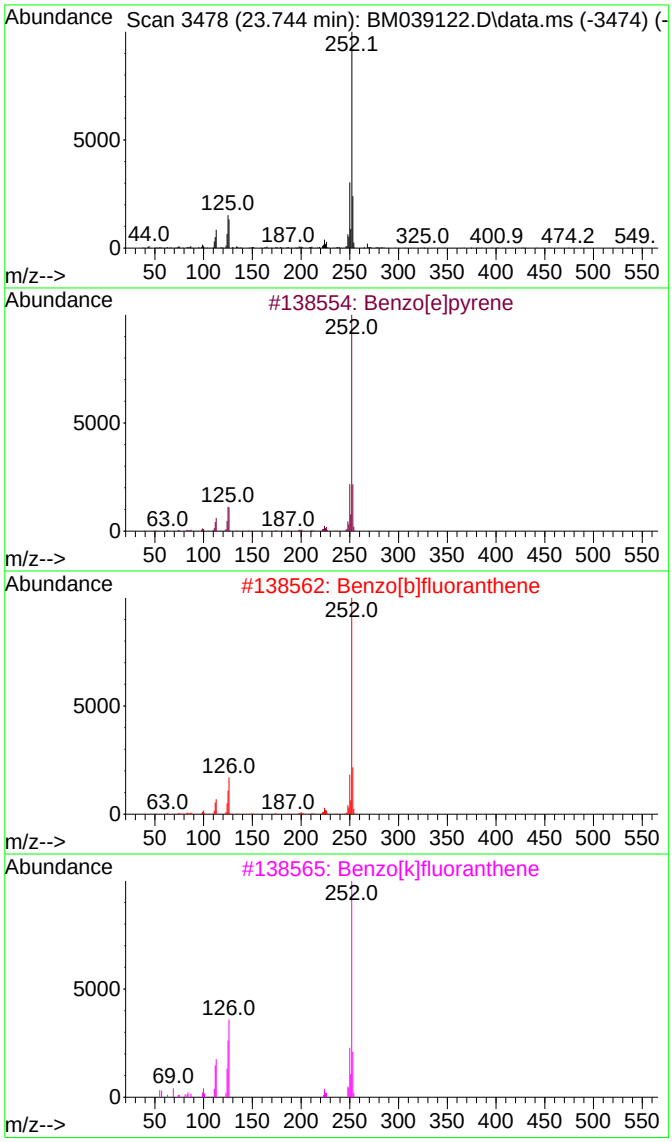
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

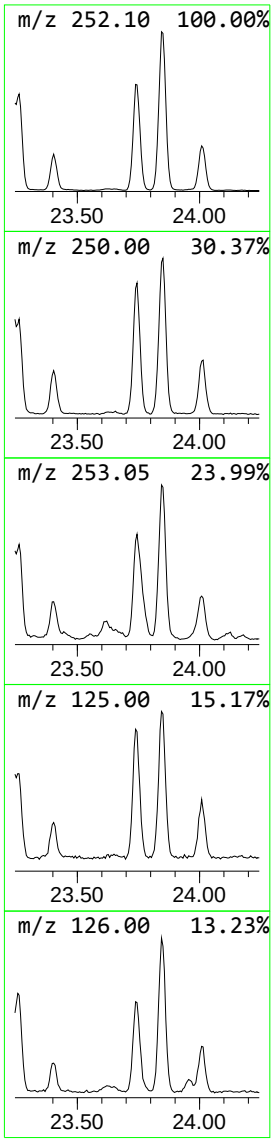
****

Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.744	7.92 ng	1157390	Perylene-d12	23.962

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032323\
Data File : BM039122.D
Acq On : 23 Mar 2023 18:48
Operator : CG/JU
Sample : 02045-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC2-20230322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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-...	5.051	38.9	ng	2958670	1	7.957	1522450	20.0
Benzene, 2-prop...	7.610	2.6	ng	194604	1	7.957	1522450	20.0
Benzene, 1-prop...	8.498	2.3	ng	174709	1	7.957	1522450	20.0
Benzophenone	15.957	5.7	ng	700115	3	14.598	2471860	20.0
n-Hexadecanoic ...	18.239	11.0	ng	1469210	4	17.345	2667210	20.0
4H-Cyclopenta[d...	18.421	3.1	ng	415605	4	17.345	2667210	20.0
Octadecanoic acid	19.515	3.3	ng	756043	5	21.527	4587420	20.0
Pentadecafluoro...	21.227	3.9	ng	891304	5	21.527	4587420	20.0
Benzo[e]pyrene	23.744	7.9	ng	1157390	6	23.962	2923350	20.0