LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132769.D
Acq On : 13 Mar 2023 19:56
Operator : CG\JU
Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.598	338	342	350	rVB	68873	81723	1.75%	0.214%
2	5.204	439	445	454	rBV	1932321	2347620	50.40%	6.134%
3	5.598	509	512	528	rVB	3374948	3450068	74.07%	9.015%
4	5.987	574	578	584	rBV	105429	104032	2.23%	0.272%
5	6.598	678	682	685	rBV	3596328	3428203	73.60%	8.957%
6	6.969	741	745	749	rBV	1490264	1160066	24.91%	3.031%
7	7.533	837	841	844	rBV	2762892	2327738	49.97%	6.082%
8	8.251	960	963	966	rBV	1942667	1583130	33.99%	4.136%
9	9.327	1142	1146	1149	rBV	5121489	4281653	91.92%	11.187%
10	10.010	1258	1262	1266	rBV	2251231	1906835	40.94%	4.982%
11	10.721	1380	1383	1387	rVB	1049897	875964	18.81%	2.289%
12	10.804	1393	1397	1401	rBV	3237057	2975203	63.87%	7.774%
13	11.504	1512	1516	1519	rBV	2418653	2116081	45.43%	5.529%
14	11.527	1519	1520	1524	rVB	230723	133378	2.86%	0.348%
15	12.016	1599	1603	1605	rBV2	251260	268509	5.76%	0.702%
16	12.121	1617	1621	1623	rBV2	90031	101690	2.18%	0.266%
17	12.557	1692	1695	1699	rBV2	70744	85070	1.83%	0.222%
18	12.598	1699	1702	1707	rVB2	43817	63191	1.36%	0.165%
19	12.651	1707	1711	1718	rVB	94051	121121	2.60%	0.316%
20	12.721	1718	1723	1727	rBV	400133	366865	7.88%	0.959%
21	12.957	1756	1763	1768	rBV	613173	628621	13.50%	1.642%
22	13.092	1782	1786	1789	rBV	5019342	4657896	100.00%	12.170%
23	13.168	1795	1799	1807	rBV3	59170	105399	2.26%	0.275%
24	13.263	1811	1815	1816	rBV3	49982	58652	1.26%	0.153%
25	13.386	1832	1836	1839	rBV2	85430	89672	1.93%	0.234%
26	13.480	1849	1852	1855	rBV	76157	70596	1.52%	0.184%
27	13.515	1855	1858	1861	rVV	73393	64252	1.38%	0.168%
28	13.645	1876	1880	1883	rBV2	66831	82566	1.77%	0.216%
29	13.798	1903	1906	1909	rVB	45433	49267	1.06%	0.129%
30	13.910	1920	1925	1927	rBV2	44133	58826	1.26%	0.154%
31	13.974	1931	1936	1949	rBV3	389722	640377	13.75%	1.673%
32	14.115	1957	1960	1962	rVB	64405	50497	1.08%	0.132%
33	14.157	1962	1967	1970	rBV	1485140	1477089	31.71%	3.859%
34	14.186	1970	1972	1978	rVB	138527	122487	2.63%	0.320%
35	14.245	1978	1982	1985	rBV	230772	214341	4.60%	0.560%
36	14.909	2091	2095	2101	rBV3	295383	336792	7.23%	0.880%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132769.D
Acq On : 13 Mar 2023 19:56
Operator : CG\JU
Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.004	2107	2111	2114	rVB	115355	123928	2.66%	0.324%
38	15.233	2146	2150	2154	rBV	108611	167610	3.60%	0.438%
39	15.556	2202	2205	2212	rVB	73596	85358	1.83%	0.223%
40	15.621	2213	2216	2221	rVB	101903	128410	2.76%	0.336%
41	15.692	2222	2228	2233	rBV2	980617	1281604	27.51%	3.349%

Sum of corrected areas: 38272380

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132769.D
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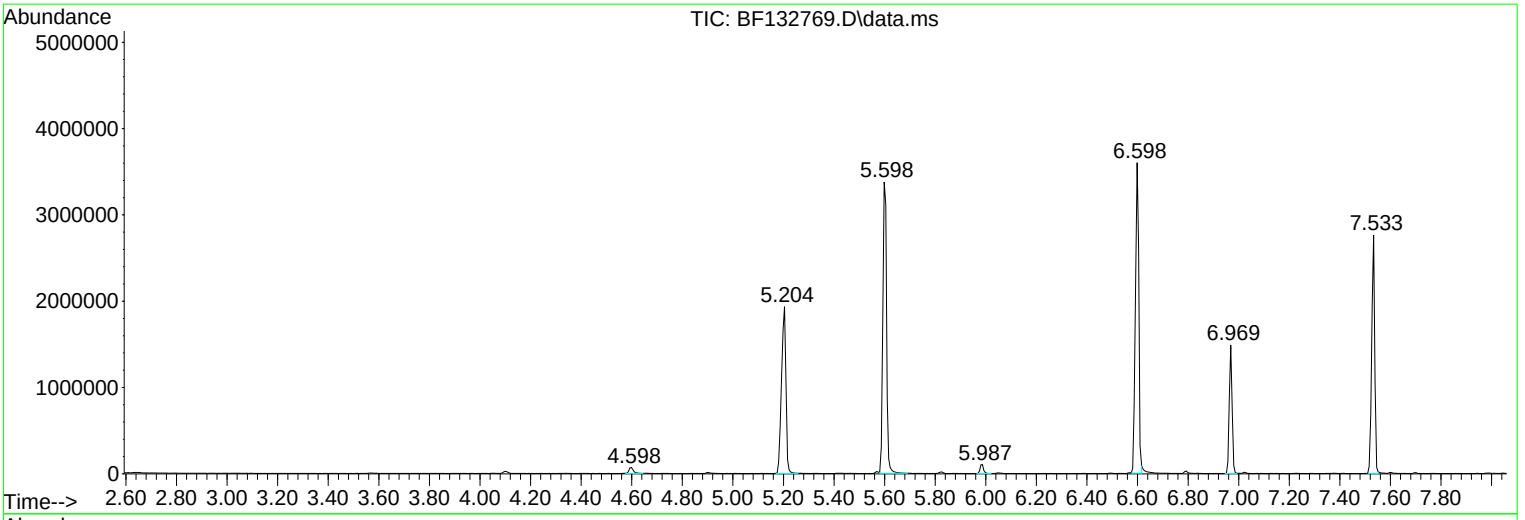
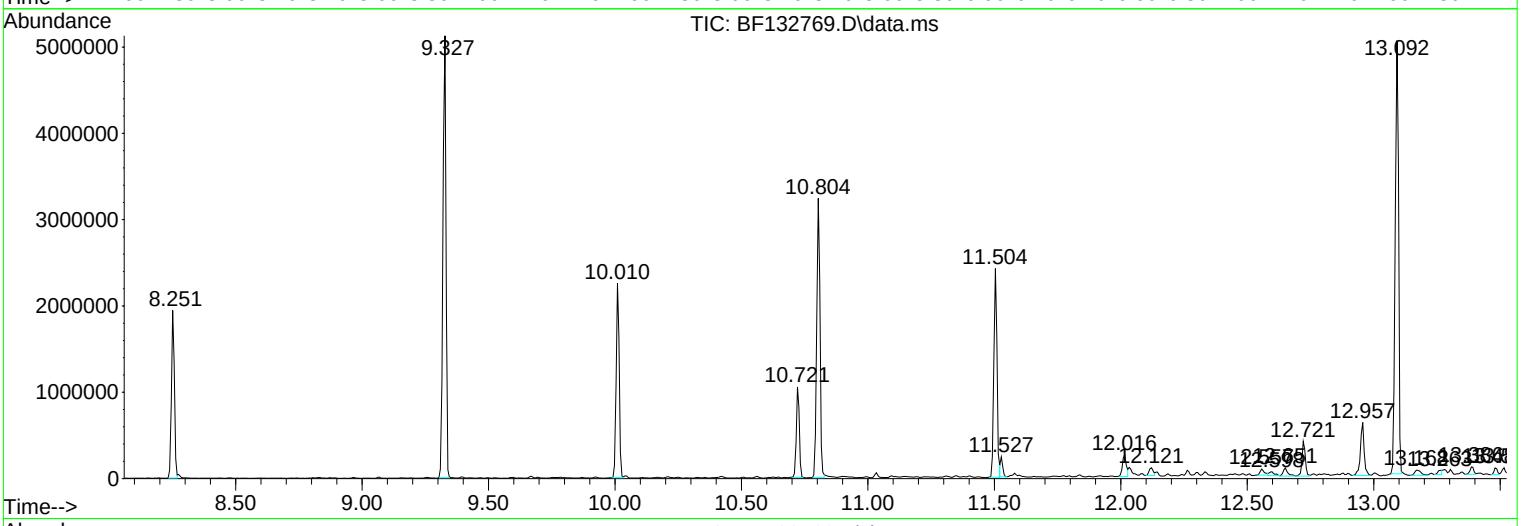
Operator : CG\JU
Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

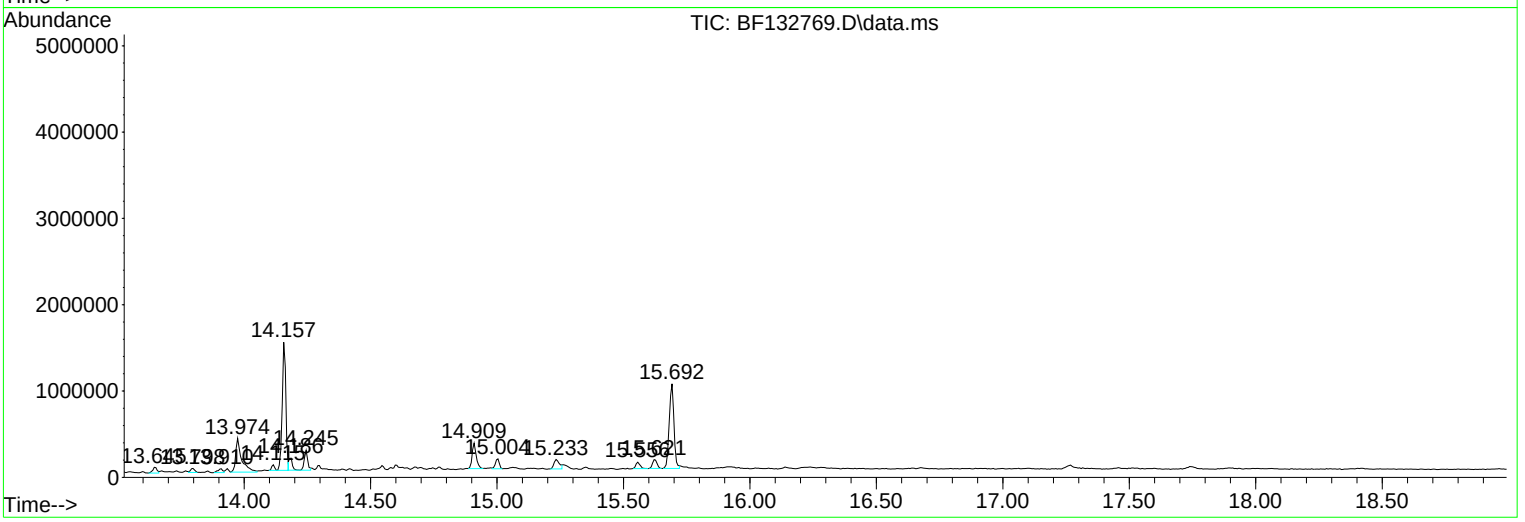
Instrument :
BNA_F
ClientSampleId :
030923-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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\BF031323\
Data File : BF132769.D
Acq On : 13 Mar 2023 19:56
Operator : CG\JU
Sample : 01863-01
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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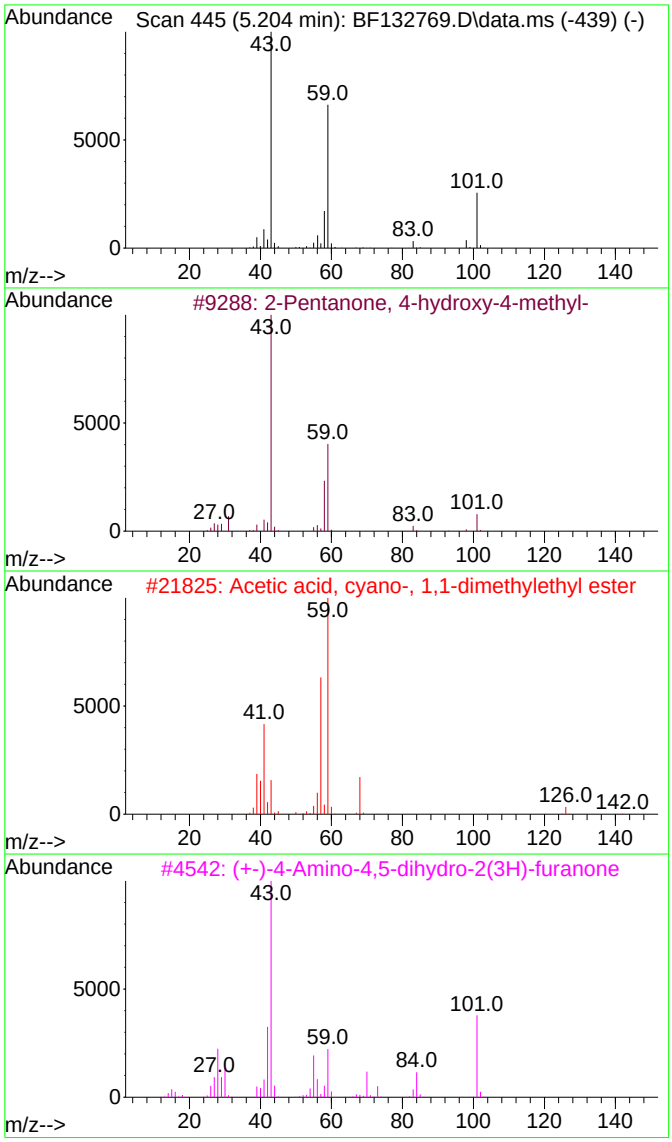
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

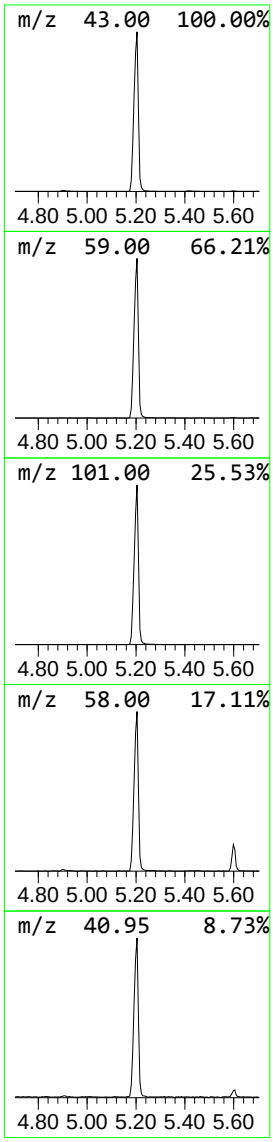
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	40.47 ng	2347620	1,4-Dichlorobenzene-d4	6.969

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	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Operator : CG\JU
Sample : 01863-01
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

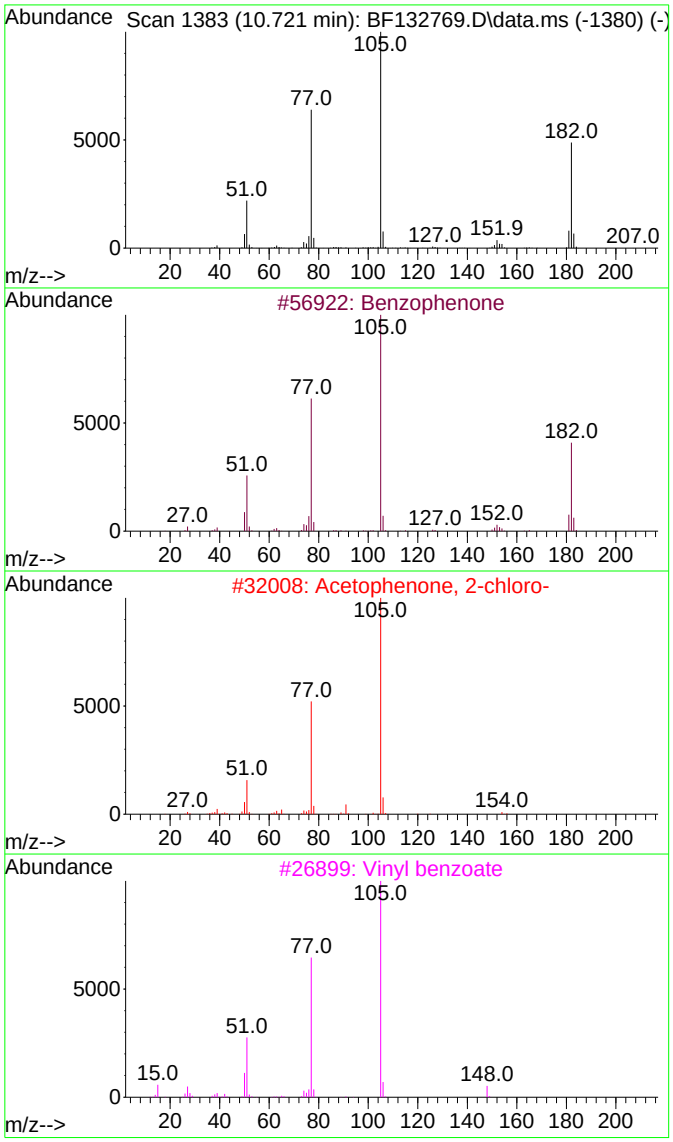
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

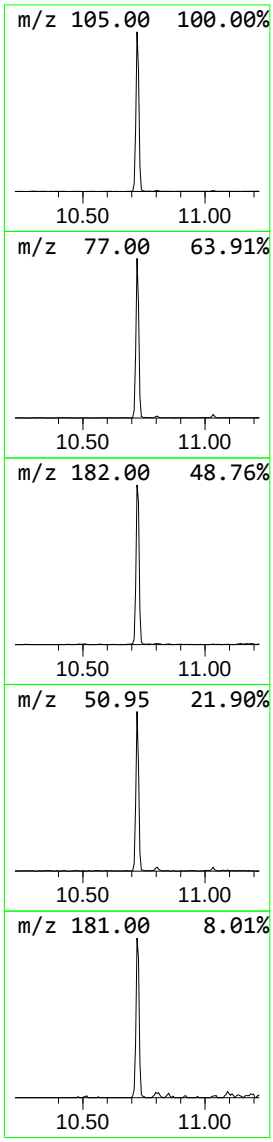
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	9.19 ng	875964	Acenaphthene-d10	10.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzilamide	227	C14H13NO2	004746-87-6	47
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132769.D
Acq On : 13 Mar 2023 19:56
Operator : CG\JU
Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

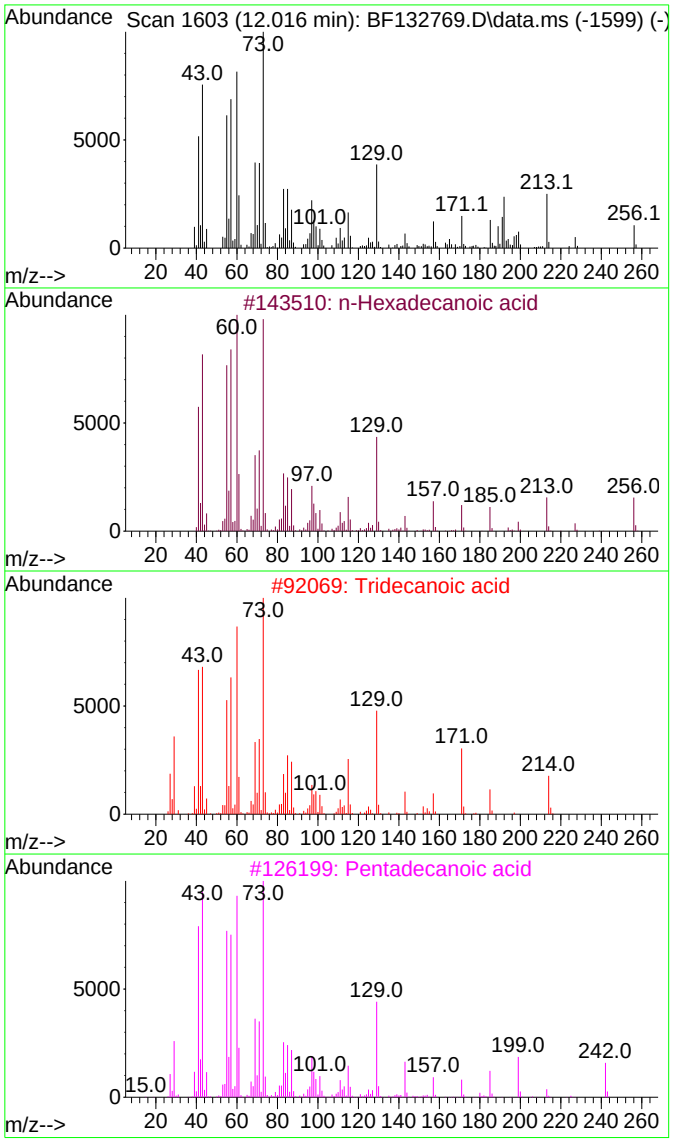
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

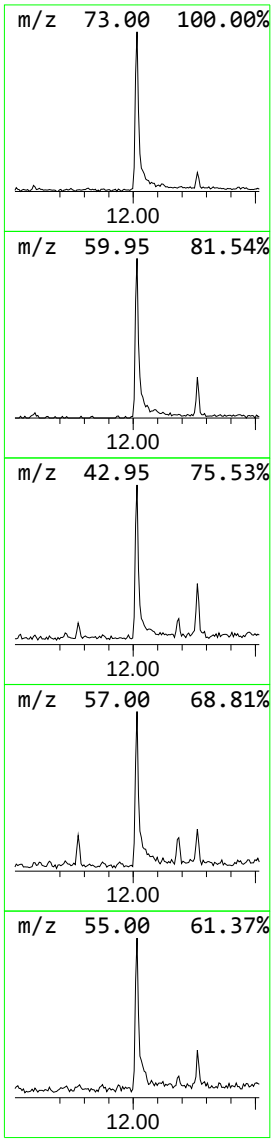
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	2.54 ng	268509	Phenanthrene-d10	11.504

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
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Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

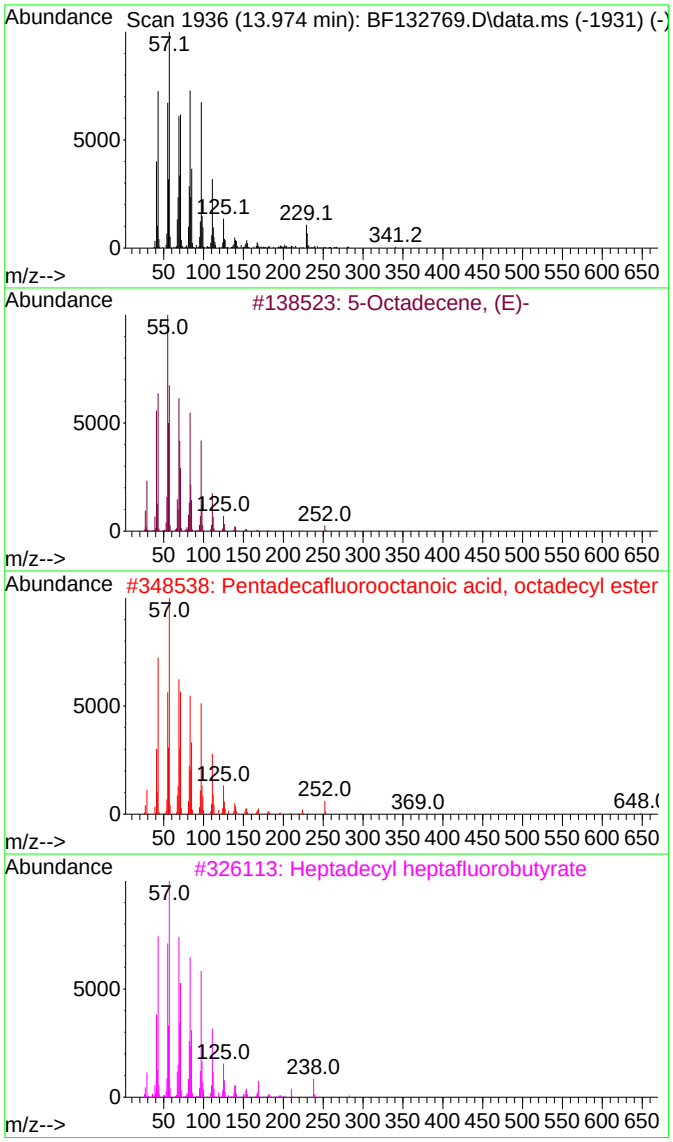
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

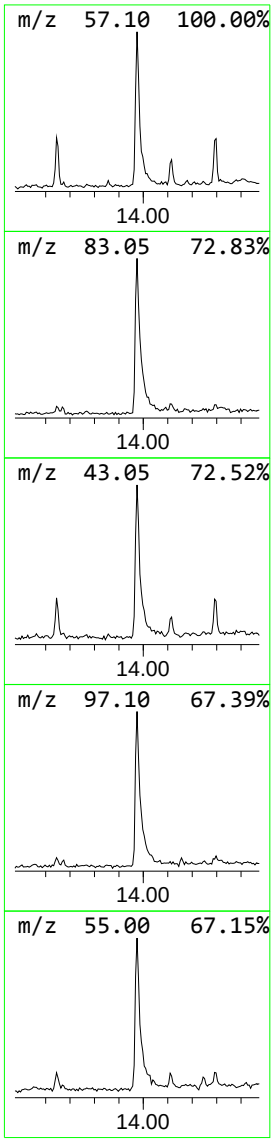
****

Peak Number 4 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	8.67 ng	640377	Chrysene-d12	14.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

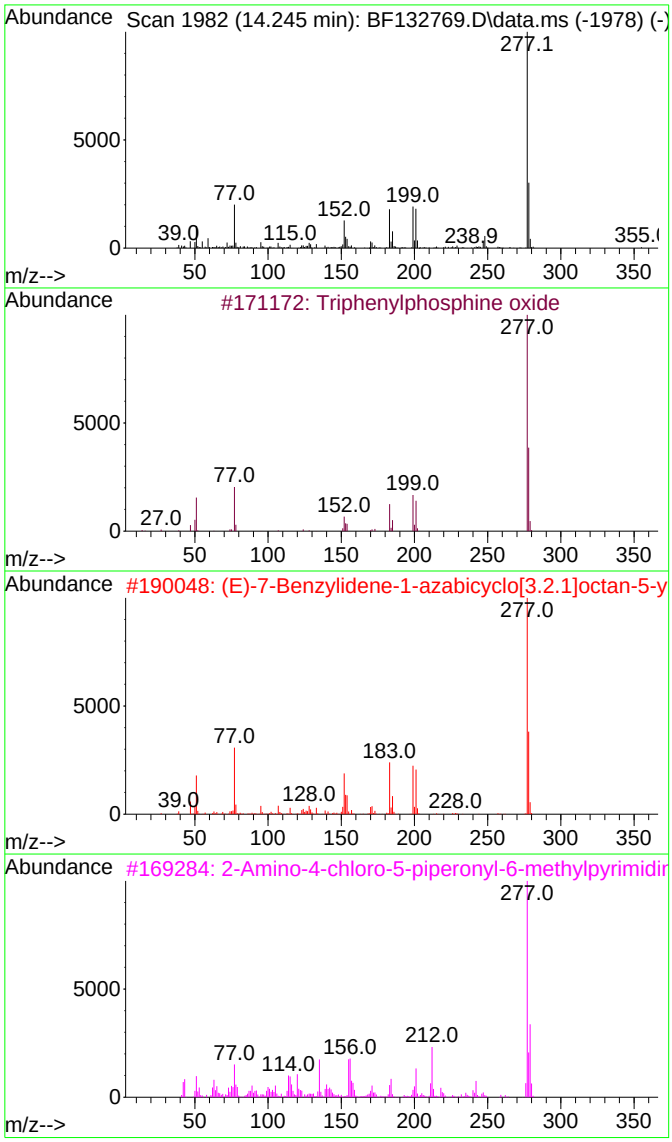
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

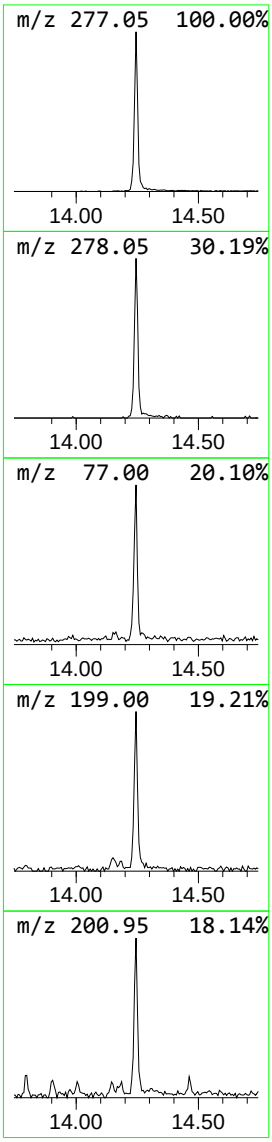
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	2.90 ng	214341	Chrysene-d12	14.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
3	2-Amino-4-chloro-5-piperonyl-6-m...	277	C13H12ClN3O2	1010257-38-4	47
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43





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Acq On : 13 Mar 2023 19:56
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Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

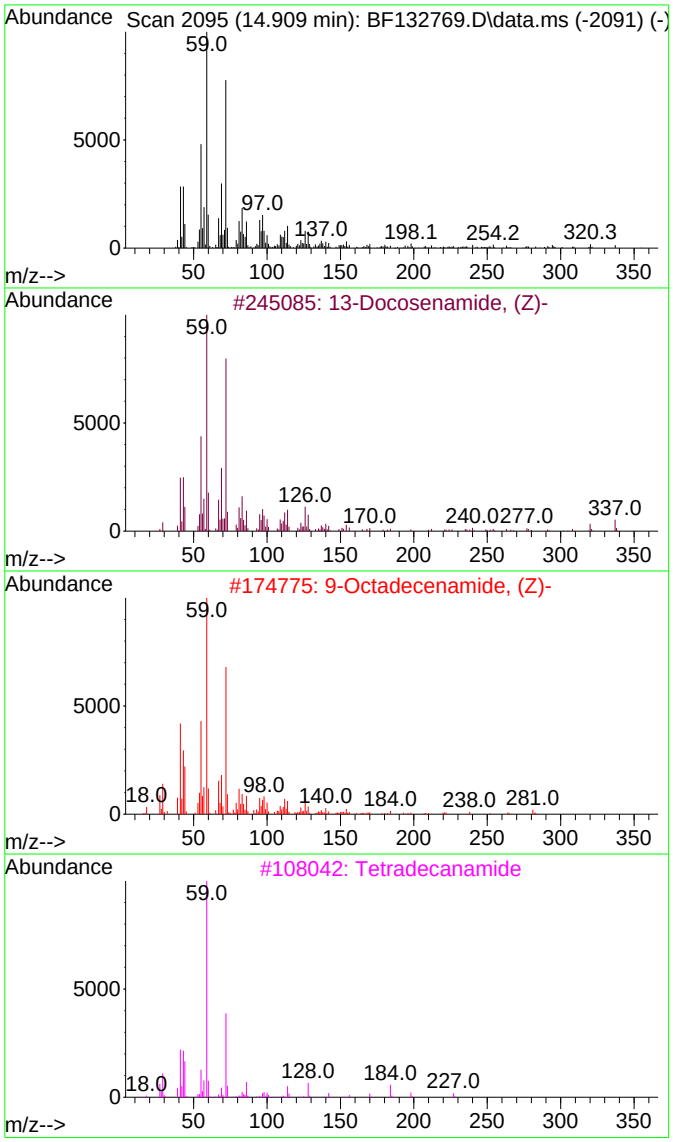
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

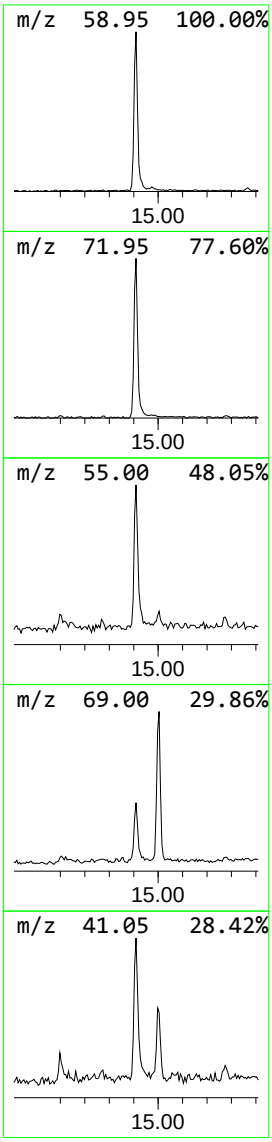
****

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	4.56 ng	336792	Chrysene-d12	14.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Tetradecanamide	227	C14H29NO	000638-58-4	47
4	Decanamide-	171	C10H21NO	002319-29-1	47
5	Dodecanamide	199	C12H25NO	001120-16-7	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

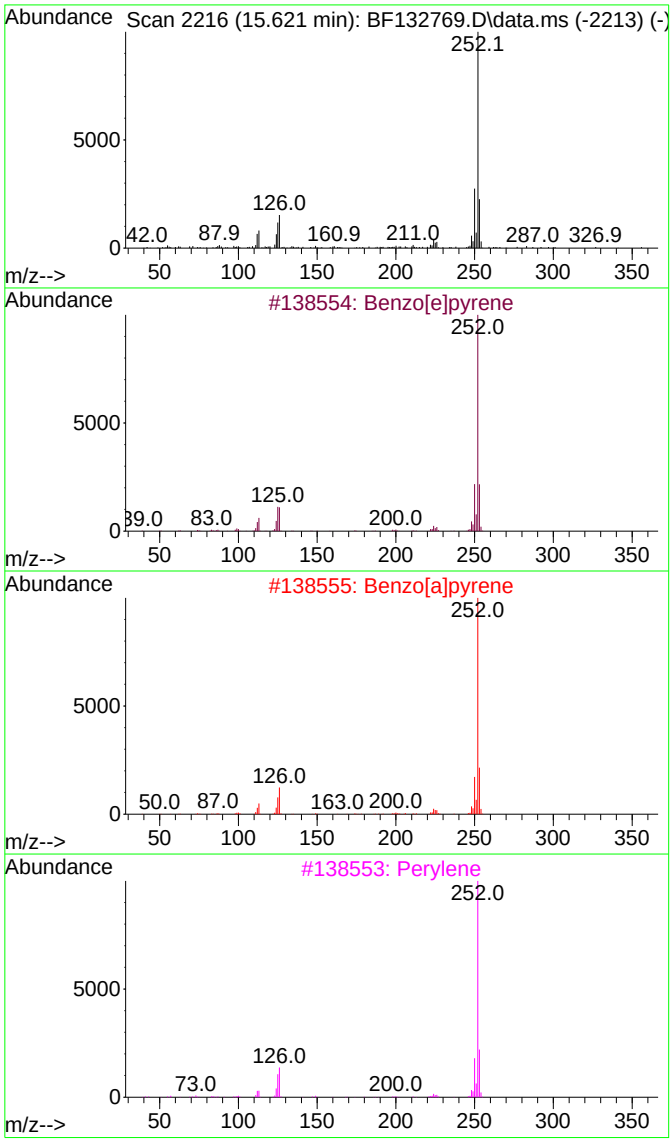
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

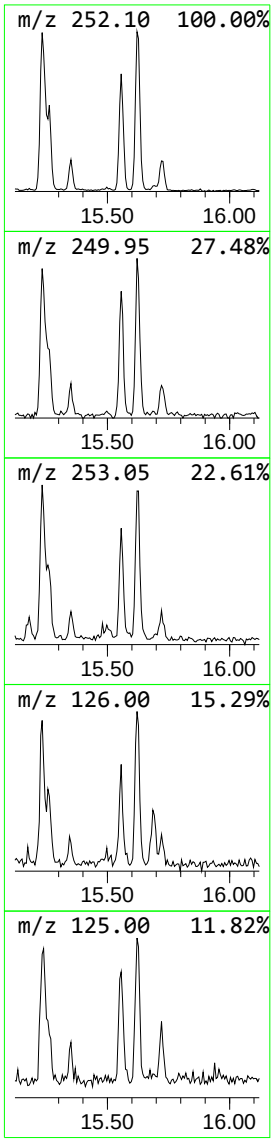
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.621	2.00 ng	128410	Perylene-d12	15.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031323\
Data File : BF132769.D
Acq On : 13 Mar 2023 19:56
Operator : CG\JU
Sample : 01863-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
030923-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.204	40.5	ng	2347620	1	6.969	1160070	20.0
Benzophenone	10.722	9.2	ng	875964	3	10.010	1906840	20.0
n-Hexadecanoic ...	12.015	2.5	ng	268509	4	11.504	2116080	20.0
5-Octadecene, (E)-	13.974	8.7	ng	640377	5	14.156	1477090	20.0
Triphenylphosph...	14.245	2.9	ng	214341	5	14.156	1477090	20.0
13-Docosenamide...	14.910	4.6	ng	336792	5	14.156	1477090	20.0
Benzo[e]pyrene	15.621	2.0	ng	128410	6	15.692	1281600	20.0