LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

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_G\Methods\8270-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.371	304	312	322	rBV	29641	52116	3.40%	0.542%
2	5.858	388	395	413	rBV	404288	708822	46.30%	7.370%
3	7.491	663	673	689	rBV	412001	780779	51.00%	8.118%
4	8.337	811	817	825	rVB	115914	197215	12.88%	2.050%
5	9.518	1010	1018	1031	rBV	279180	507941	33.18%	5.281%
6	11.174	1293	1300	1306	rBV	155325	283554	18.52%	2.948%
7	11.221	1306	1308	1315	rVB	16370	24642	1.61%	0.256%
8	12.808	1571	1578	1584	rBV	20304	32451	2.12%	0.337%
9	13.019	1608	1614	1620	rVB2	15168	25210	1.65%	0.262%
10	13.577	1700	1709	1718	rBV	770553	1194436	78.02%	12.419%
11	14.123	1795	1802	1809	rBV3	7159	16256	1.06%	0.169%
12	14.270	1822	1827	1832	rBV2	13674	25163	1.64%	0.262%
13	14.329	1832	1837	1840	rVV4	11353	17859	1.17%	0.186%
14	14.388	1842	1847	1851	rVB5	10293	16381	1.07%	0.170%
15	14.676	1891	1896	1902	rBV4	8429	16280	1.06%	0.169%
16	14.793	1913	1916	1922	rVB	12503	17733	1.16%	0.184%
17	14.952	1937	1943	1950	rVB	230818	363040	23.71%	3.775%
18	15.016	1950	1954	1960	rVB3	9406	16309	1.07%	0.170%
19	15.345	2003	2010	2017	rBV2	18224	32441	2.12%	0.337%
20	15.410	2017	2021	2028	rVB5	9865	16964	1.11%	0.176%
21	15.739	2065	2077	2084	rBV6	18637	43620	2.85%	0.454%
22	15.980	2112	2118	2120	rBV3	11519	19773	1.29%	0.206%
23	16.285	2160	2170	2176	rVB2	33374	55173	3.60%	0.574%
24	16.438	2190	2196	2202	rBV	531018	798089	52.13%	8.298%
25	16.597	2220	2223	2225	rBV3	17636	23631	1.54%	0.246%
26	16.620	2225	2227	2230	rVB	16635	17853	1.17%	0.186%
27	17.055	2296	2301	2306	rBV7	8855	21246	1.39%	0.221%
28	17.213	2323	2328	2332	rBV7	9549	18083	1.18%	0.188%
29	17.348	2345	2351	2355	rBV3	17819	34384	2.25%	0.358%
30	17.695	2403	2410	2414	rBV	278994	449813	29.38%	4.677%
31	17.736	2414	2417	2423	rVB	108735	150788	9.85%	1.568%
32	17.824	2428	2432	2440	rVV	22095	39188	2.56%	0.407%
33	18.100	2473	2479	2480	rBV3	14275	22905	1.50%	0.238%
34	18.124	2480	2483	2488	rVB3	17269	25265	1.65%	0.263%
35	18.277	2503	2509	2512	rBV7	15563	27309	1.78%	0.284%
36	18.529	2547	2552	2555	rBV	61081	88034	5.75%	0.915%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

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_G\Methods\8270-BG052723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.606	2561	2565	2570	rVB	44035	69692	4.55%	0.725%
38	18.747	2583	2589	2594	rBV4	35112	93310	6.10%	0.970%
39	19.046	2637	2640	2645	rVB	24288	34074	2.23%	0.354%
40	19.105	2646	2650	2655	rVB2	22634	39469	2.58%	0.410%
41	19.457	2707	2710	2713	rVB	25452	31427	2.05%	0.327%
42	19.728	2750	2756	2760	rBV	273670	392887	25.66%	4.085%
43	20.051	2807	2811	2813	rBV2	42038	58165	3.80%	0.605%
44	20.086	2813	2817	2823	rVB	264317	379097	24.76%	3.942%
45	20.262	2841	2847	2856	rBV	1216181	1530883	100.00%	15.917%
46	21.995	3134	3142	3147	rBV3	261933	640576	41.84%	6.660%
47	22.042	3148	3150	3156	rVB	111838	167576	10.95%	1.742%

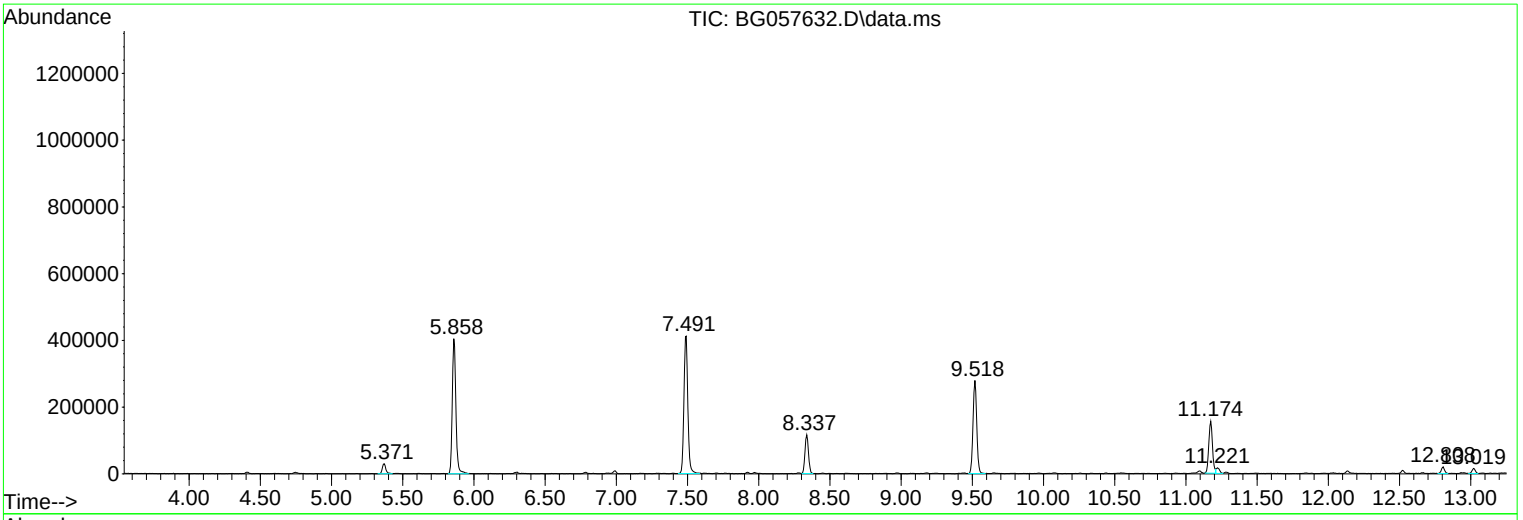
Sum of corrected areas: 9617902

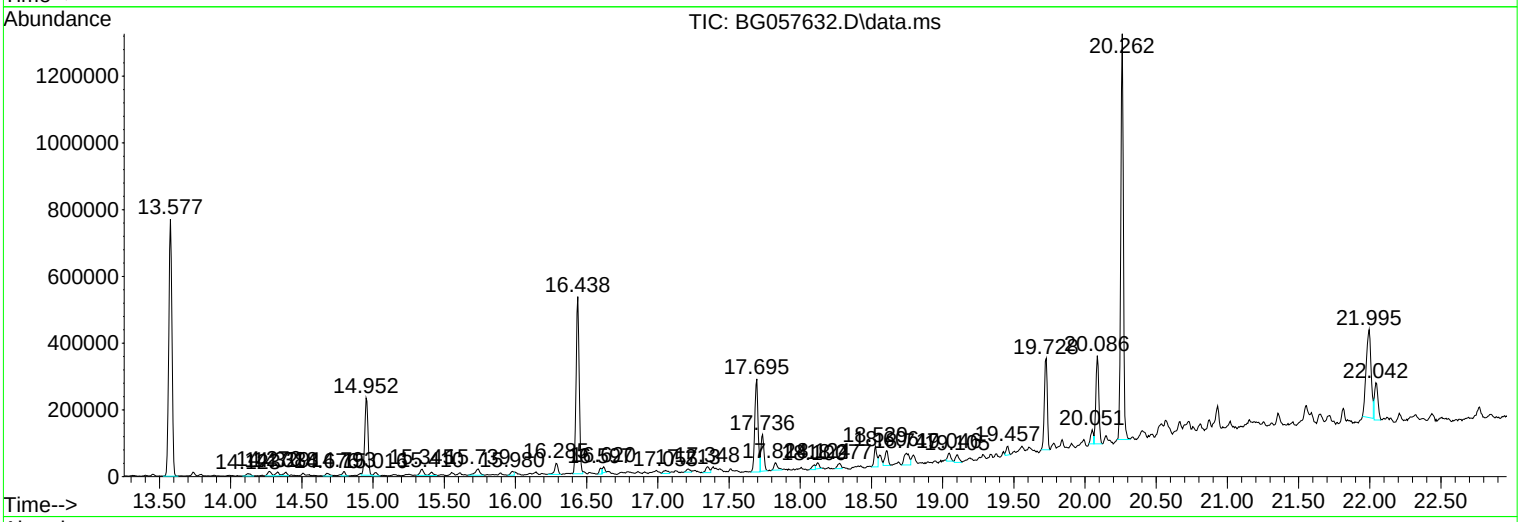
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

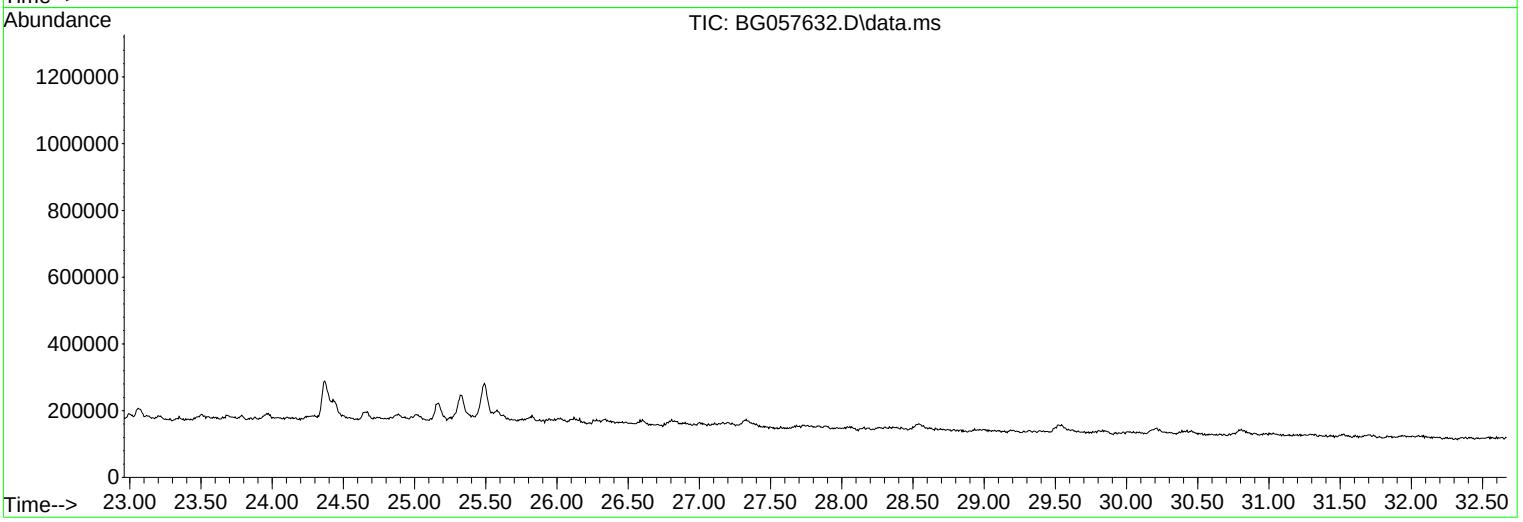
Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

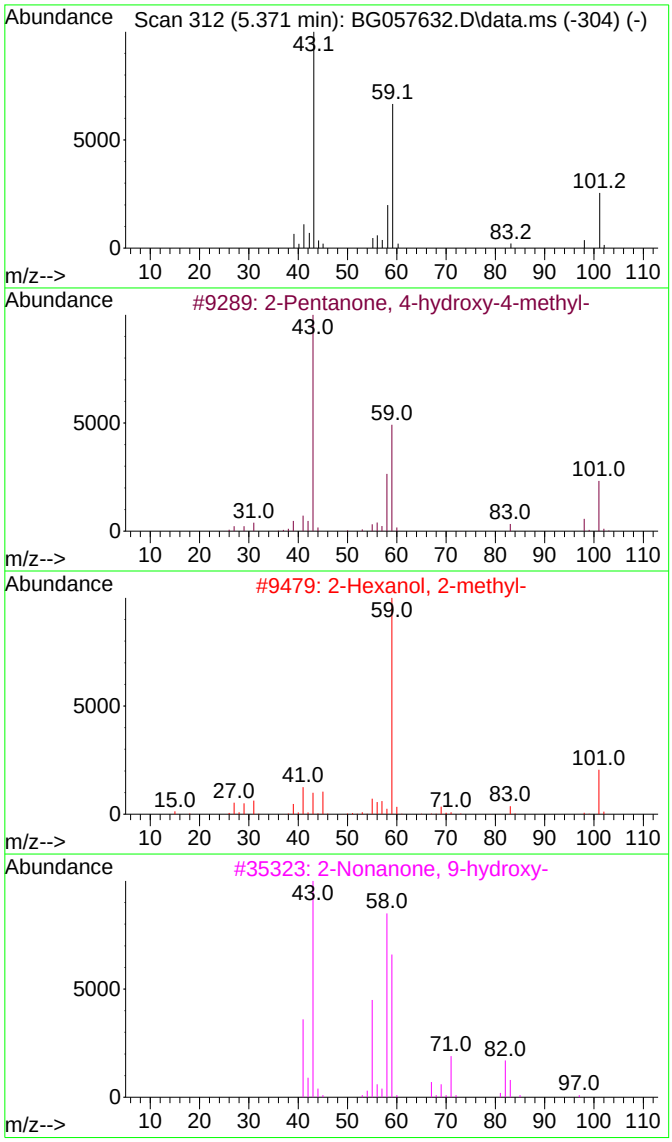
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

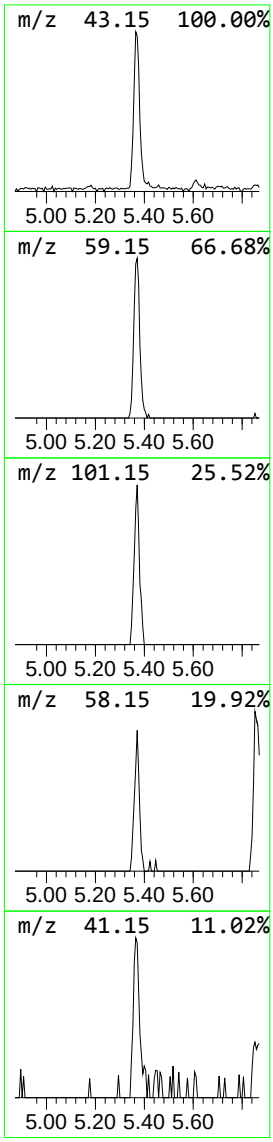
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.371	5.29 ng	52116	1,4-Dichlorobenzene-d4	8.337

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

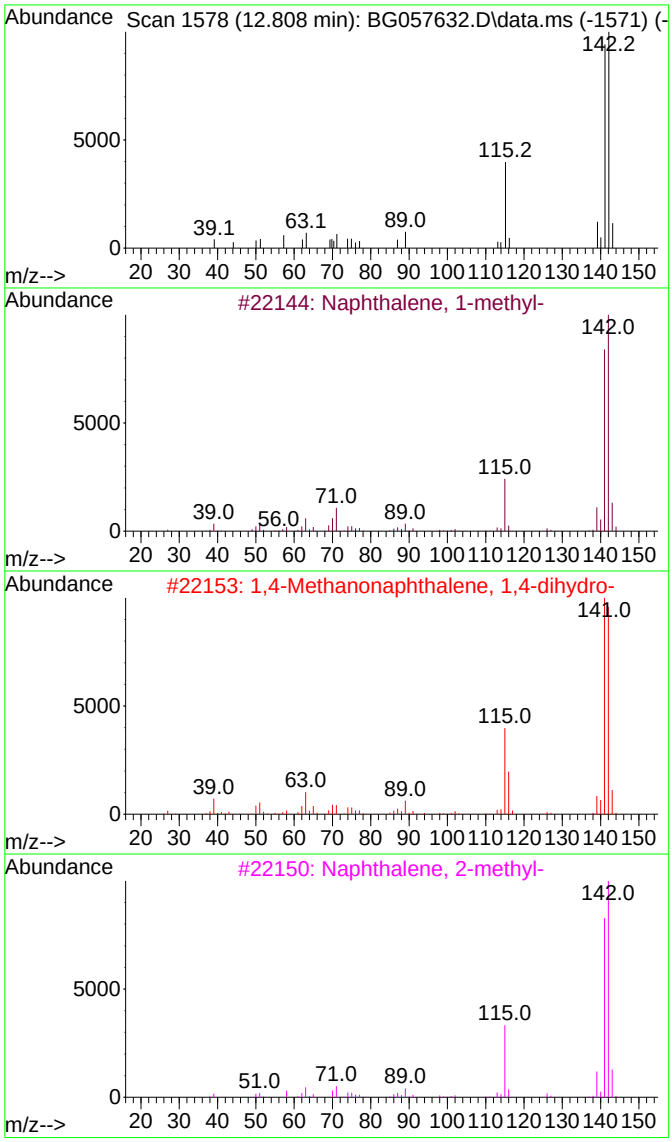
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

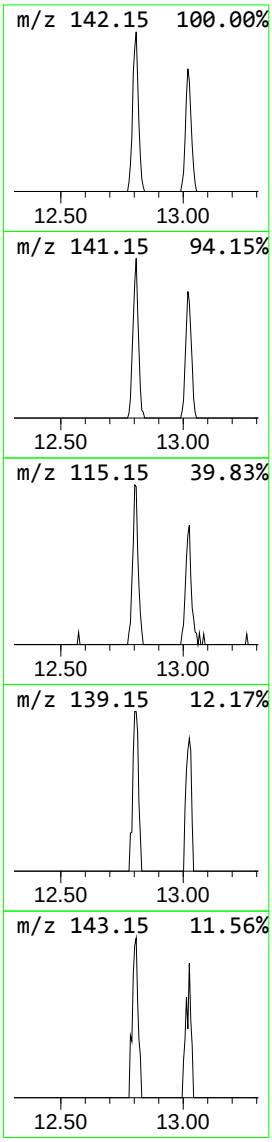
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,4-Methanonaphthalene, 1,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.807	2.29 ng	32451	Naphthalene-d8	11.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

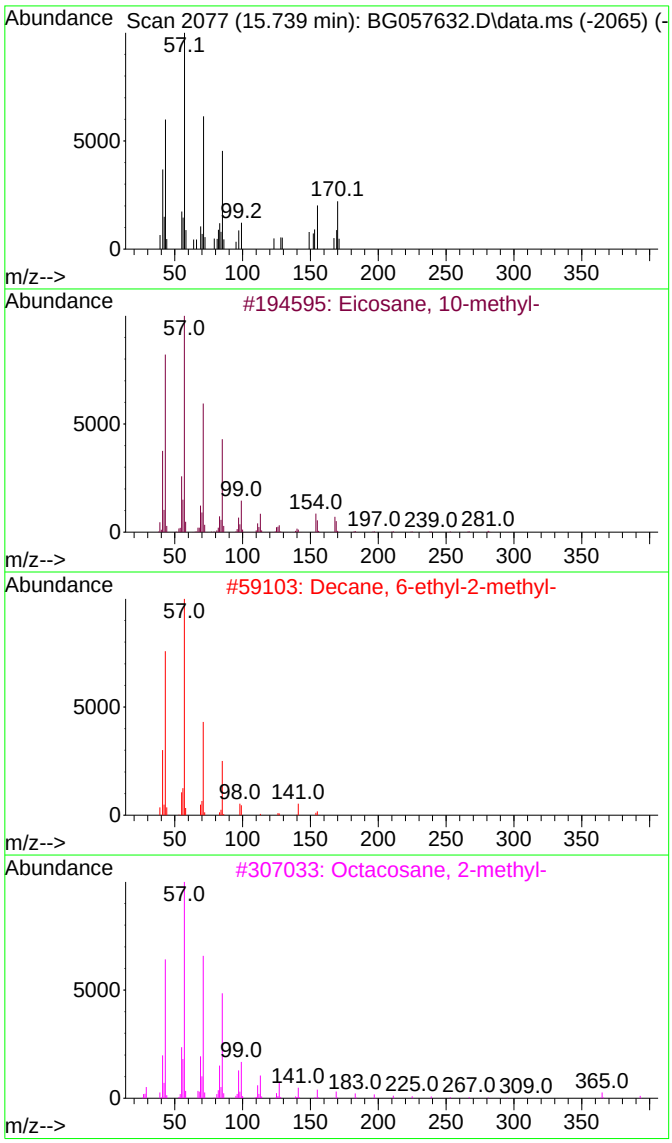
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

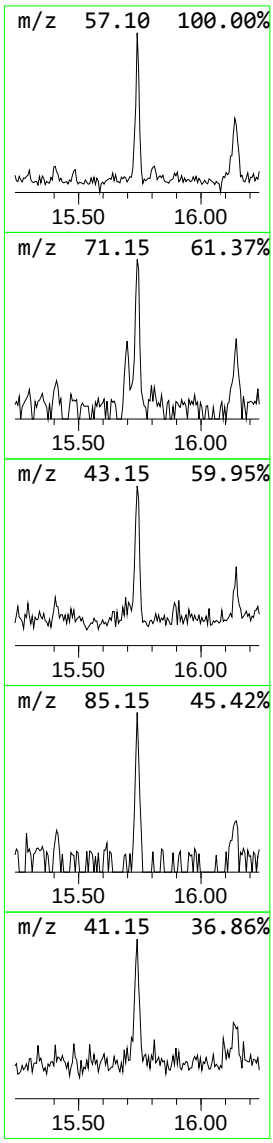
****

Peak Number 3 Eicosane, 10-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.40 ng	43620	Acenaphthene-d10	14.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	52
2	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	50
4	Octacosane	394	C28H58	000630-02-4	50
5	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

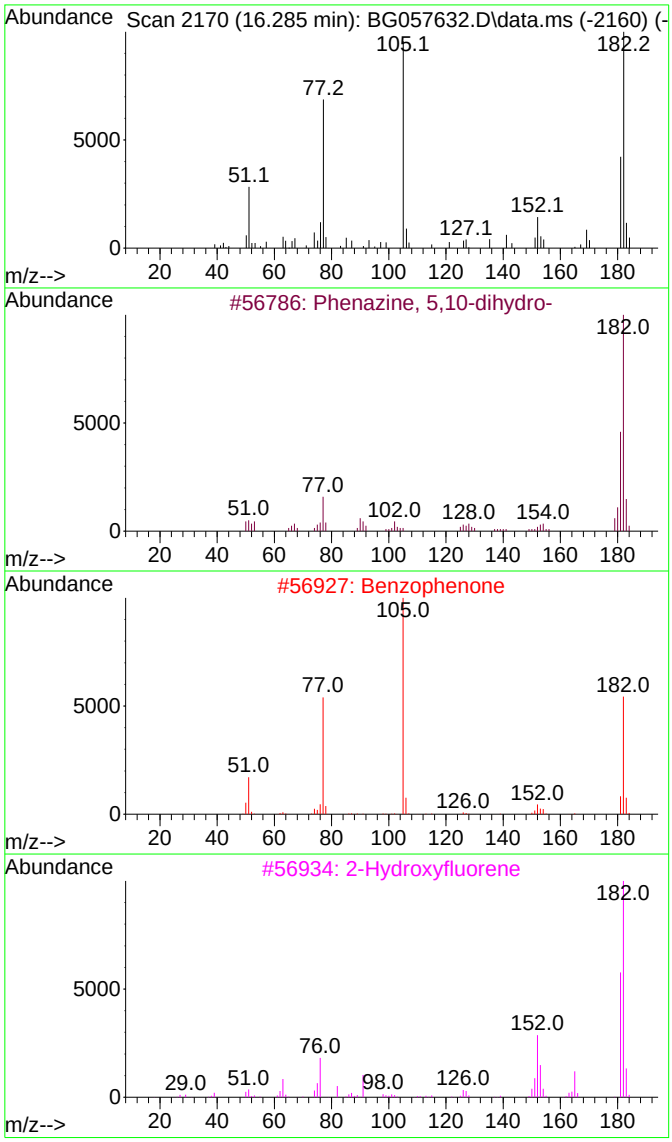
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

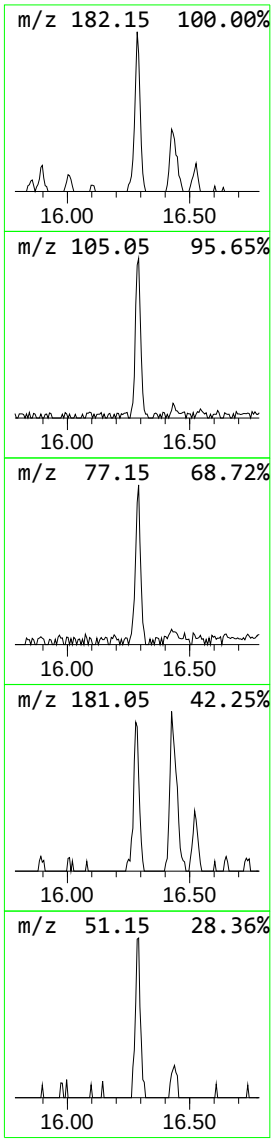
****

Peak Number 4 Phenazine, 5,10-dihydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.285	3.04 ng	55173	Acenaphthene-d10	14.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenazine, 5,10-dihydro-	182	C12H10N2	000613-32-1	64
2	Benzophenone	182	C13H10O	000119-61-9	52
3	2-Hydroxyfluorene	182	C13H10O	002443-58-5	50
4	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	49
5	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

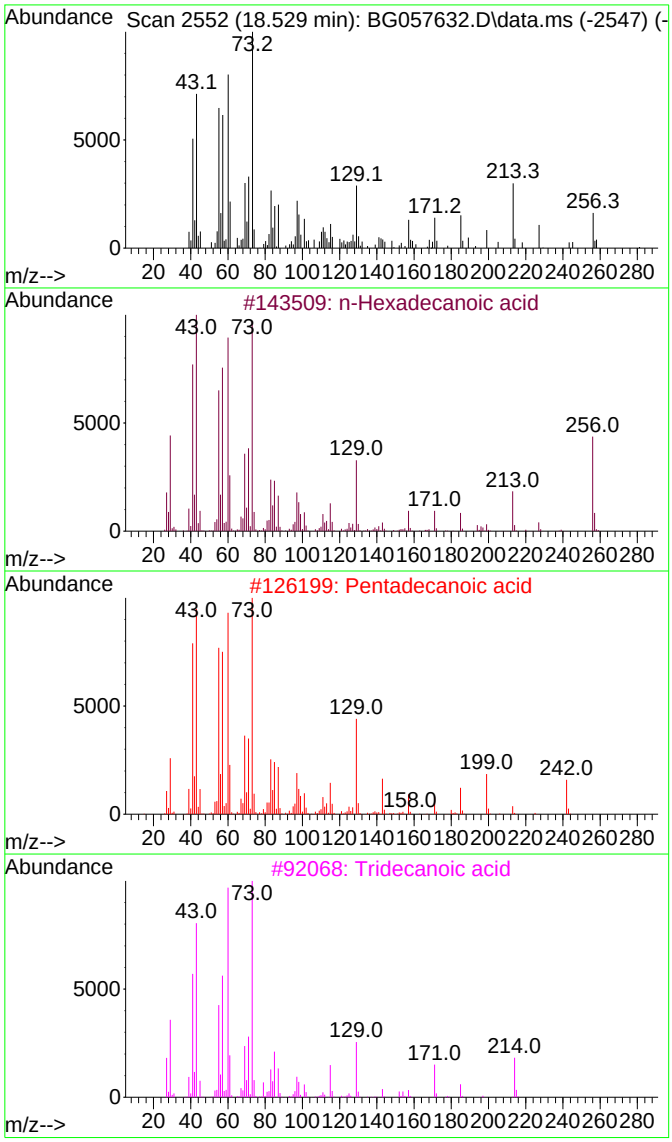
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

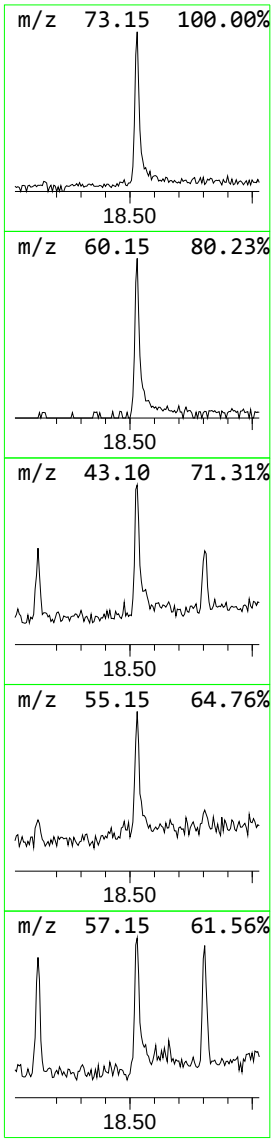
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.529	3.91 ng	88034	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	62
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

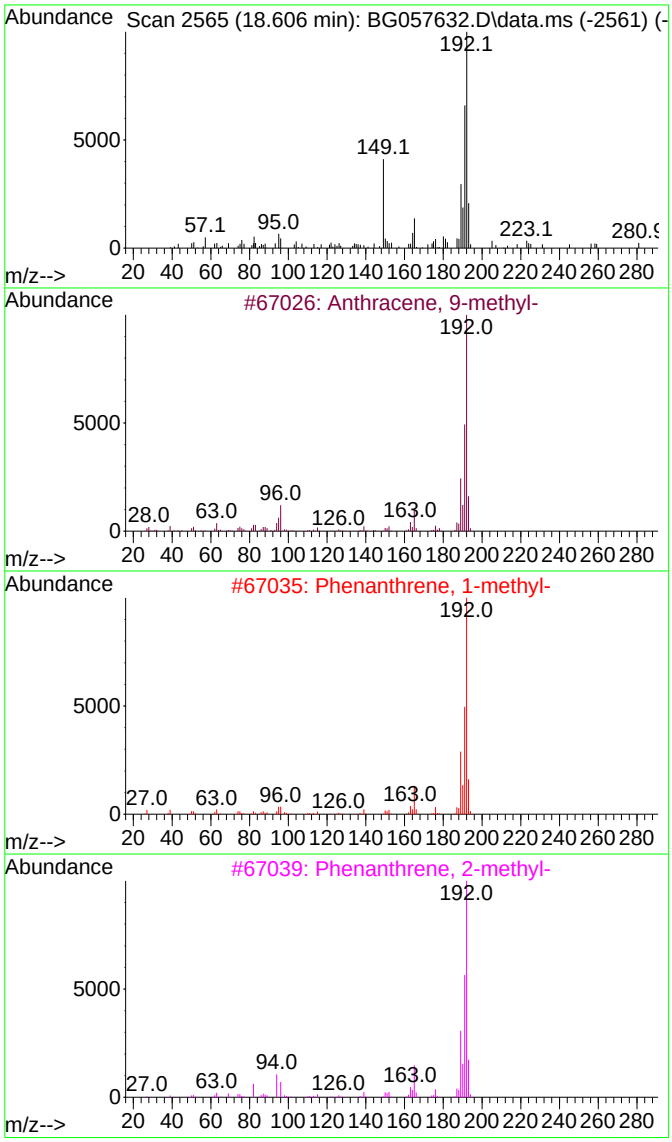
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

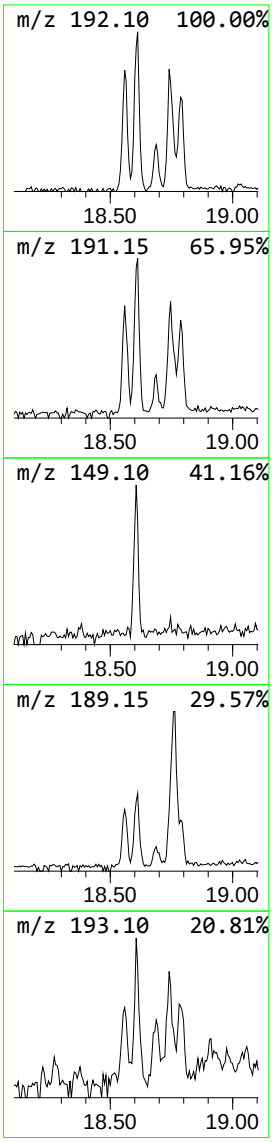
****

Peak Number 6 Anthracene, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.606	3.10 ng	69692	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

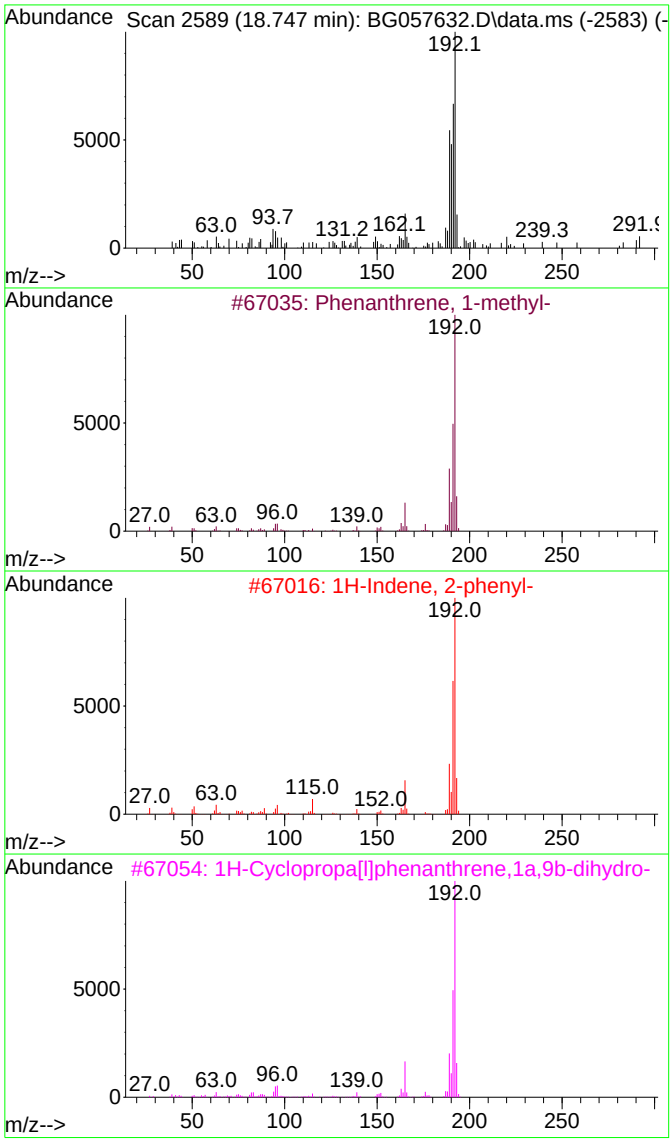
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

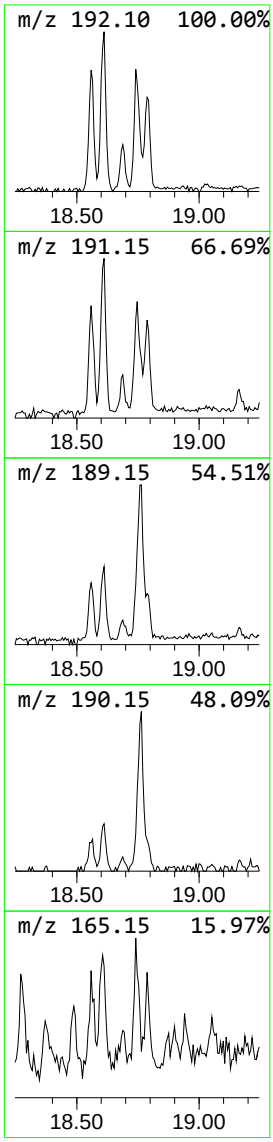
****

Peak Number 7 Phenanthrene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.747	4.15 ng	93310	Phenanthrene-d10	17.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	53
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	53
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	53
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057632.D
Acq On : 31 May 2023 22:11
Operator : CG/JU
Sample : 02979-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR044-VNJ224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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-...	5.371	5.3	ng	52116	1	8.337	197215	20.0
1,4-Methanonaph...	12.807	2.3	ng	32451	2	11.174	283554	20.0
Eicosane, 10-me...	15.739	2.4	ng	43620	3	14.952	363040	20.0
Phenazine, 5,10...	16.285	3.0	ng	55173	3	14.952	363040	20.0
n-Hexadecanoic ...	18.529	3.9	ng	88034	4	17.695	449813	20.0
Anthracene, 9-m...	18.606	3.1	ng	69692	4	17.695	449813	20.0
Phenanthrene, 1...	18.747	4.2	ng	93310	4	17.695	449813	20.0