LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054796.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.215	321	328	337	rBV	68269	110951	4.32%	0.545%
2	5.691	401	409	421	rBV	771608	1243368	48.39%	6.108%
3	7.301	674	683	694	rBV	762452	1334782	51.94%	6.557%
4	8.153	821	828	834	rBV	178375	312018	12.14%	1.533%
5	9.322	1018	1027	1039	rBV	458582	828055	32.22%	4.068%
6	10.973	1301	1308	1315	rBV	255195	461656	17.97%	2.268%
7	13.406	1715	1722	1732	rBV	1276917	1969856	76.66%	9.677%
8	14.223	1856	1861	1868	rBV	22486	35256	1.37%	0.173%
9	14.781	1945	1956	1962	rBV	402032	638106	24.83%	3.135%
10	14.845	1962	1967	1975	rVB2	74033	115291	4.49%	0.566%
11	15.174	2015	2023	2031	rBV	36063	57922	2.25%	0.285%
12	15.827	2127	2134	2145	rBV2	61904	98336	3.83%	0.483%
13	16.267	2202	2209	2218	rBV	928991	1430089	55.65%	7.025%
14	16.502	2237	2249	2257	rVB6	19921	46493	1.81%	0.228%
15	16.825	2295	2304	2309	rBV4	13699	29698	1.16%	0.146%
16	17.178	2359	2364	2372	rVB3	27212	45892	1.79%	0.225%
17	17.348	2388	2393	2399	rVB	22152	34530	1.34%	0.170%
18	17.530	2416	2424	2427	rBV	468648	744059	28.96%	3.655%
19	17.572	2427	2431	2438	rVV	365504	551591	21.47%	2.710%
20	17.660	2438	2446	2451	rVV	46632	82287	3.20%	0.404%
21	17.718	2451	2456	2464	rVB3	12015	25790	1.00%	0.127%
22	17.924	2486	2491	2499	rBV	26475	52304	2.04%	0.257%
23	18.400	2565	2572	2576	rBV	56107	88576	3.45%	0.435%
24	18.447	2576	2580	2588	rVB2	63736	106336	4.14%	0.522%
25	18.529	2589	2594	2599	rBV3	18455	29610	1.15%	0.145%
26	18.600	2599	2606	2610	rBV3	84669	168459	6.56%	0.828%
27	18.794	2634	2639	2647	rBV9	30279	51846	2.02%	0.255%
28	18.894	2651	2656	2660	rBV	37575	60488	2.35%	0.297%
29	18.935	2660	2663	2671	rVB	43583	63439	2.47%	0.312%
30	19.311	2722	2727	2732	rBV	41609	64369	2.50%	0.316%
31	19.369	2732	2737	2740	rBV5	19080	38250	1.49%	0.188%
32	19.452	2747	2751	2757	rBV3	27795	47441	1.85%	0.233%
33	19.575	2766	2772	2778	rVB	677391	949850	36.96%	4.666%
34	19.722	2793	2797	2801	rBV3	19996	32274	1.26%	0.159%
35	19.822	2810	2814	2820	rVB2	17150	33530	1.30%	0.165%
36	19.904	2821	2828	2830	rVV2	111280	216350	8.42%	1.063%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.939	2830	2834	2841	rVV	512260	758099	29.50%	3.724%
38	20.004	2841	2845	2850	rVB	29086	48587	1.89%	0.239%
39	20.127	2860	2866	2872	rBV	1972976	2569626	100.00%	12.624%
40	20.239	2881	2885	2895	rBV4	60061	165952	6.46%	0.815%
41	20.421	2913	2916	2921	rVB	96809	136866	5.33%	0.672%
42	20.521	2929	2933	2937	rBV	65816	94284	3.67%	0.463%
43	20.721	2964	2967	2971	rBV	36733	53326	2.08%	0.262%
44	21.197	3044	3048	3053	rVB	41257	67425	2.62%	0.331%
45	21.432	3084	3088	3093	rBV	200755	270572	10.53%	1.329%
46	21.684	3127	3131	3139	rVB	244492	347839	13.54%	1.709%
47	21.819	3145	3154	3159	rBV3	511838	1258531	48.98%	6.183%
48	21.866	3159	3162	3170	rVB	226691	383285	14.92%	1.883%
49	24.117	3537	3545	3552	rBV	171381	549548	21.39%	2.700%
50	24.875	3668	3674	3685	rVB2	100912	285339	11.10%	1.402%
51	25.027	3693	3700	3712	rVB2	127957	382244	14.88%	1.878%
52	25.192	3719	3728	3738	rBV2	261900	785110	30.55%	3.857%

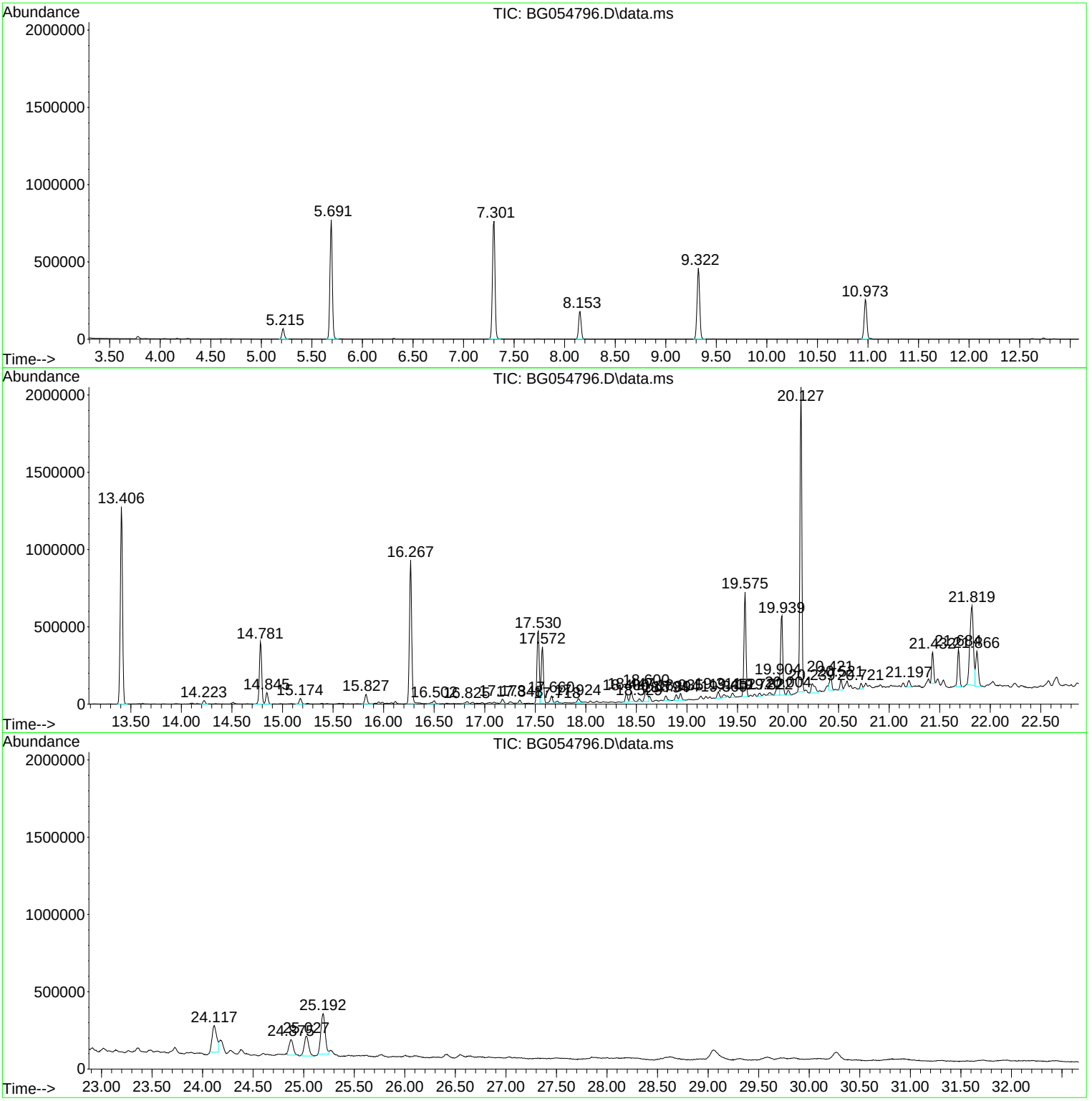
Sum of corrected areas: 20355781

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

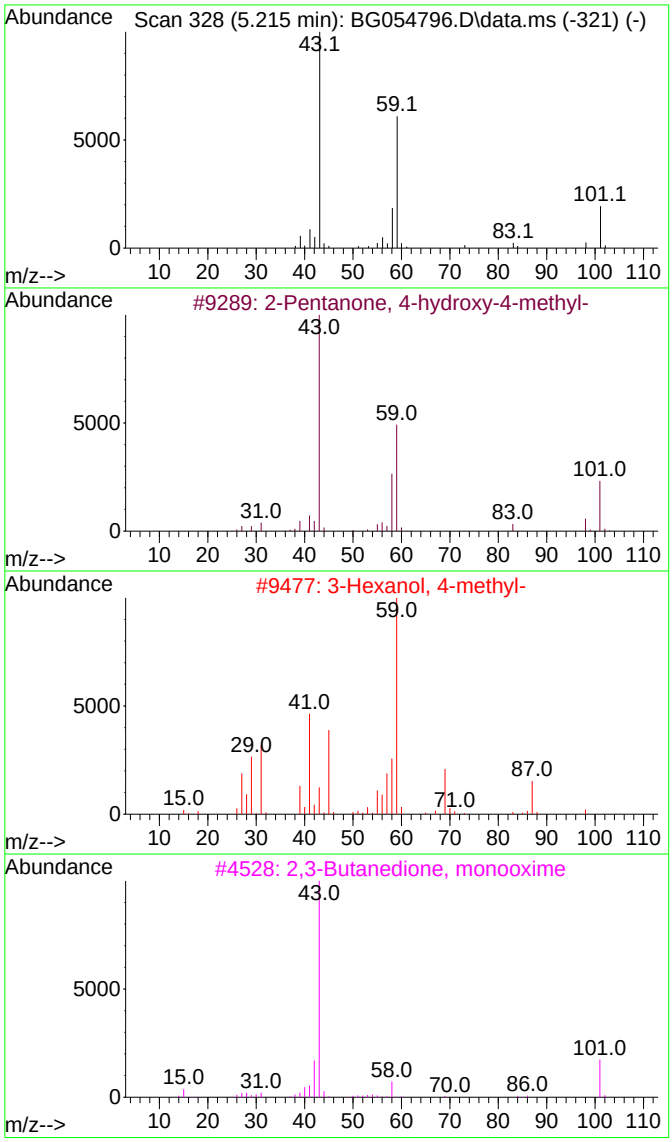
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

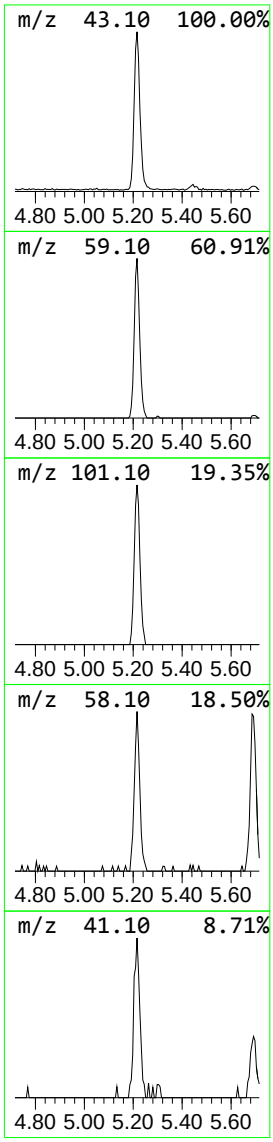
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.215	7.11 ng	110951	1,4-Dichlorobenzene-d4	8.153

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

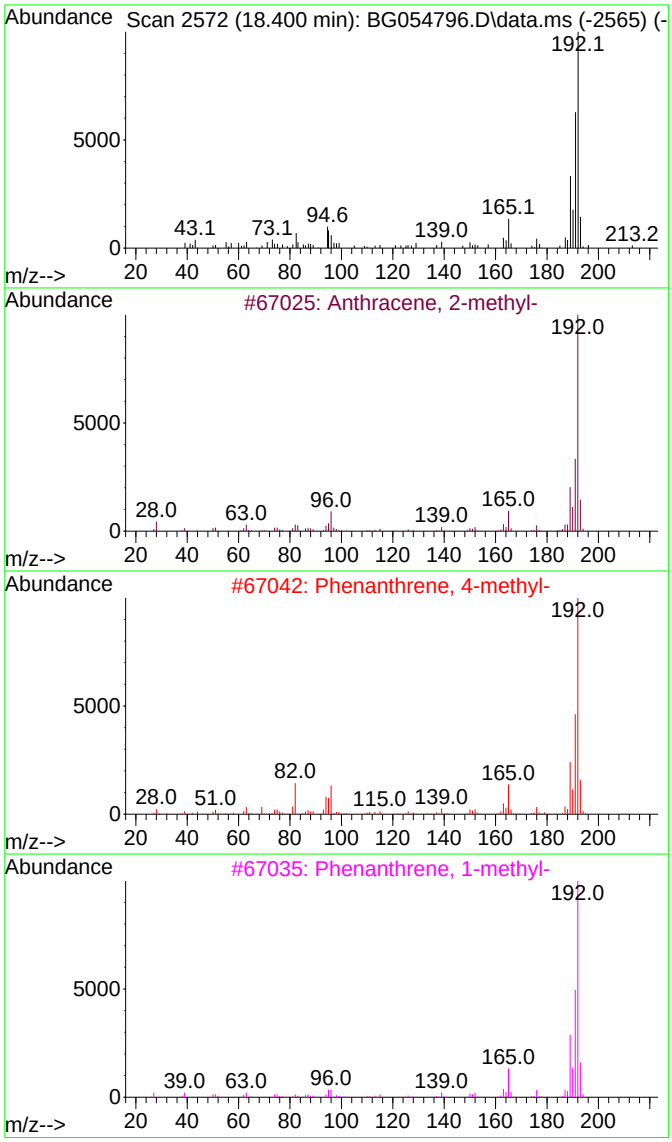
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

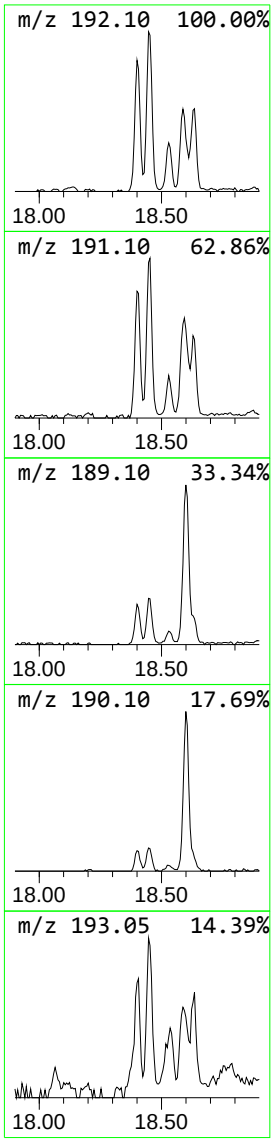
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.400	2.38 ng	88576	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

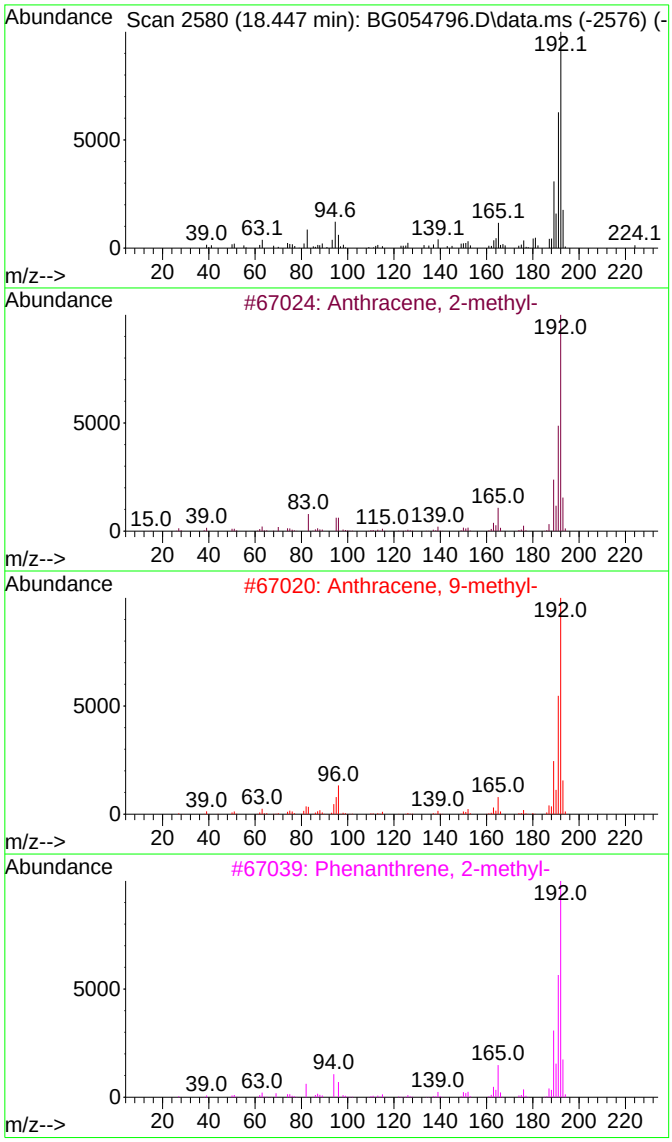
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

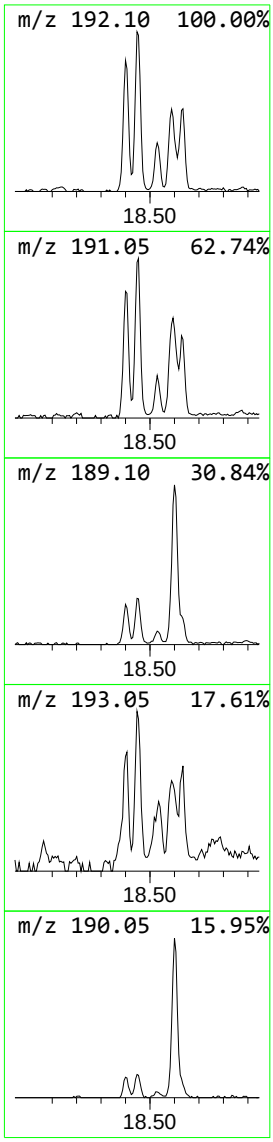
****

Peak Number 4 Anthracene, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.447	2.86 ng	106336	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

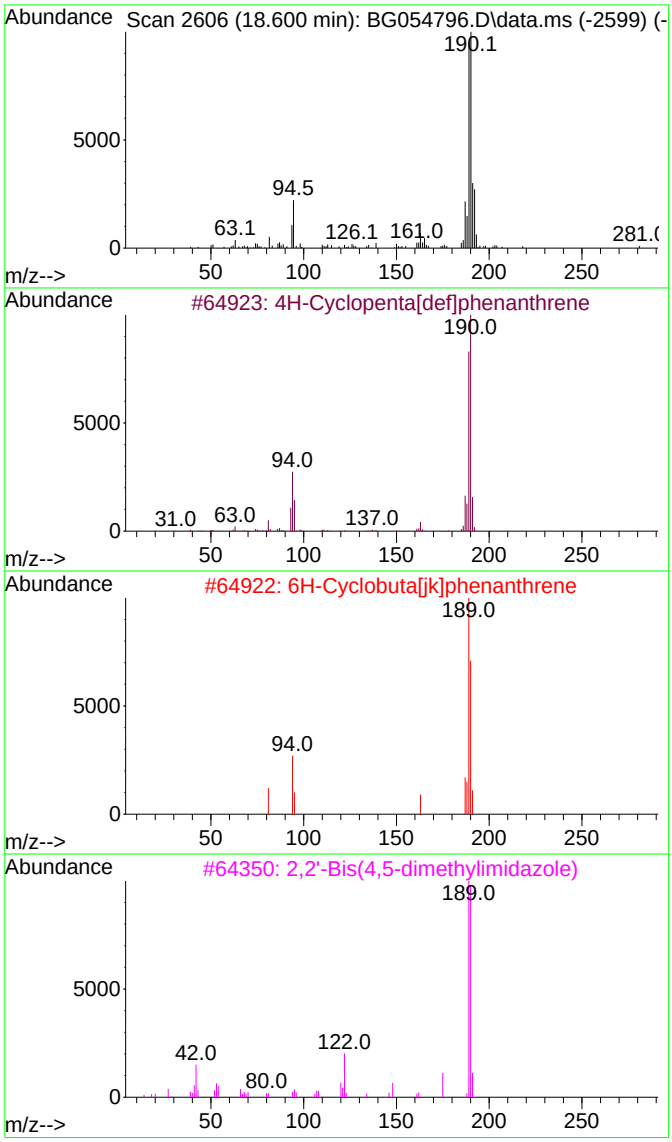
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

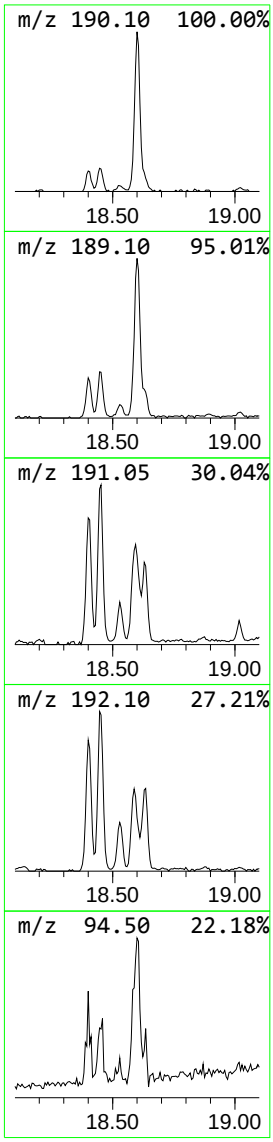
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.600	4.53 ng	168459	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

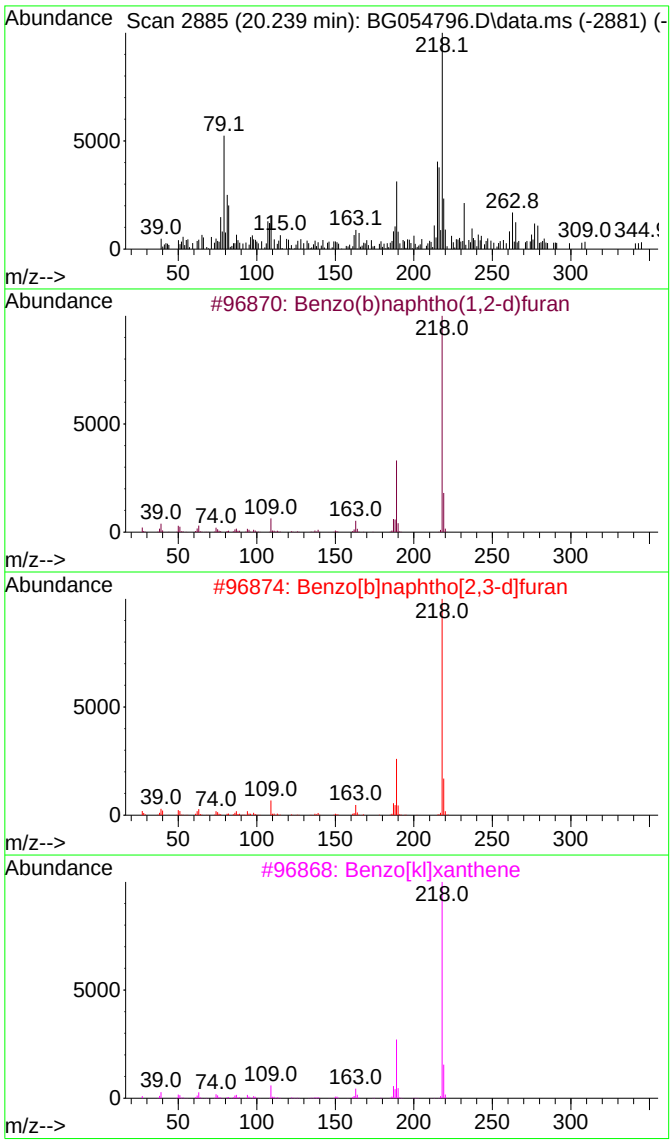
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

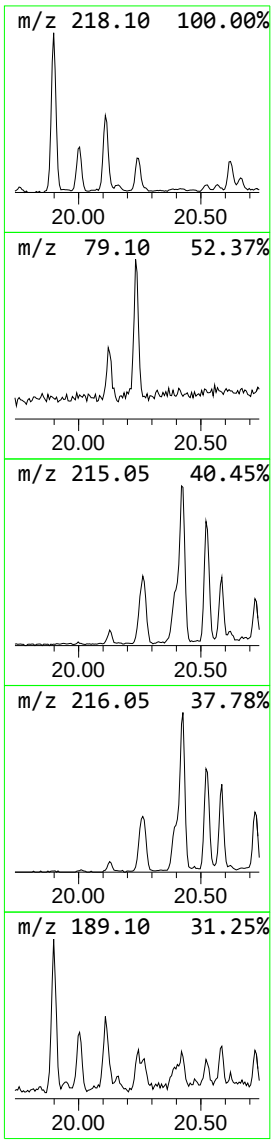
****

Peak Number 6 unknown20.239 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.239	2.64 ng	165952	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo(b)naphtho(1,2-d)furan	218	C16H10O	000205-39-0	42
2	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	42
3	Benzo[kl]xanthene	218	C16H10O	000200-23-7	42
4	1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	35
5	Alanine, 3-(p-tert-butoxyphenyl)...	381	C19H35NO3Si2	1000506-39-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

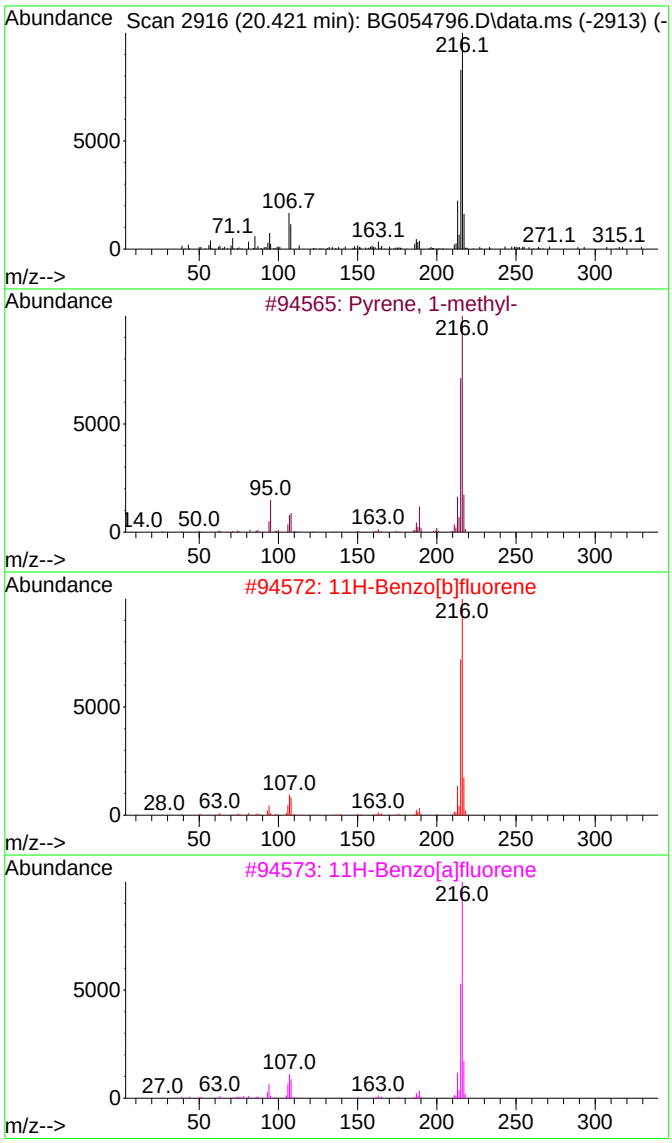
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

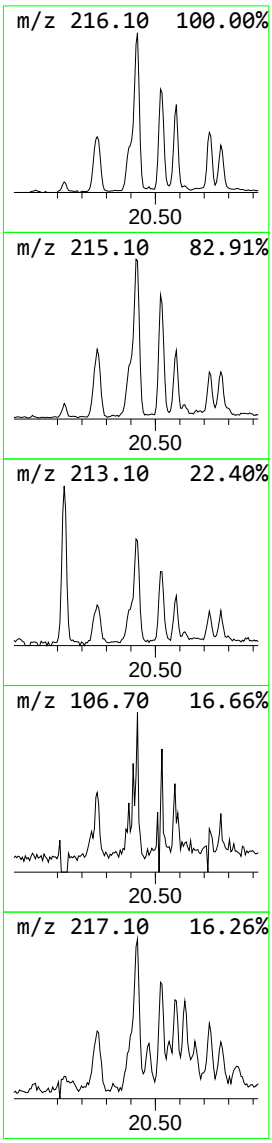
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.421	2.18 ng	136866	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

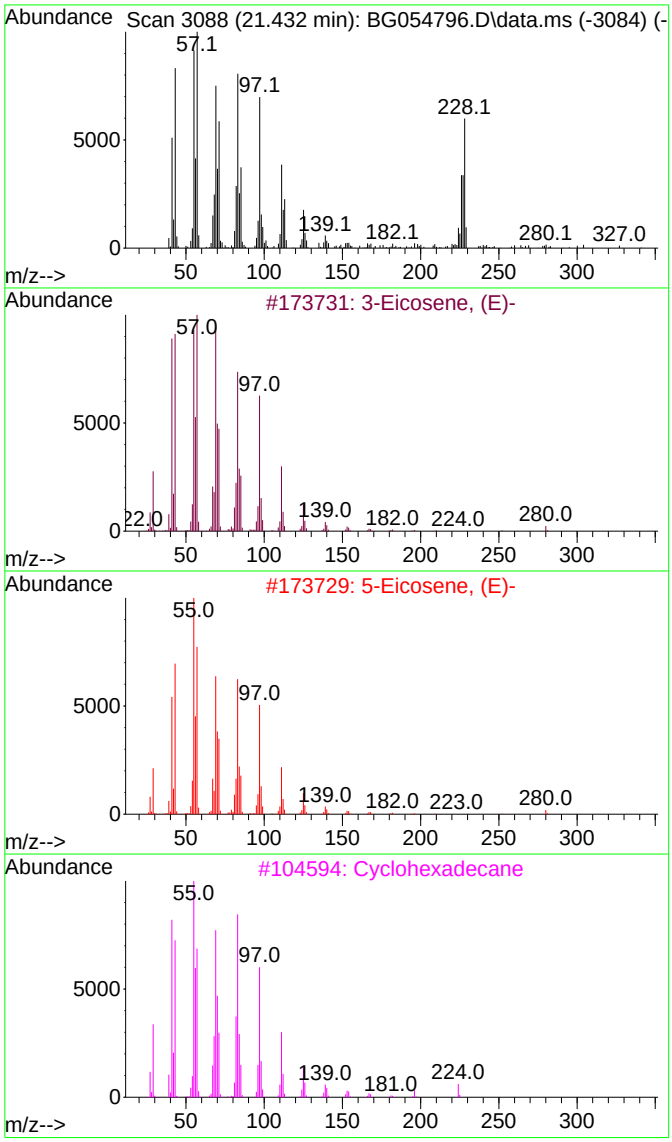
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

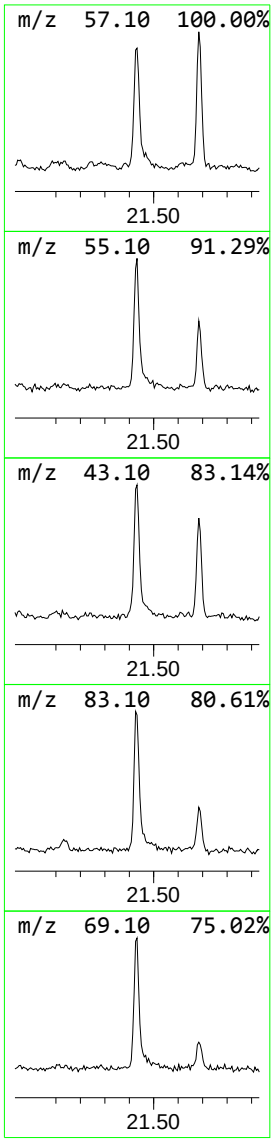
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.432	4.30 ng	270572	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	89
5	1-Hexacosene	364	C26H52	018835-33-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

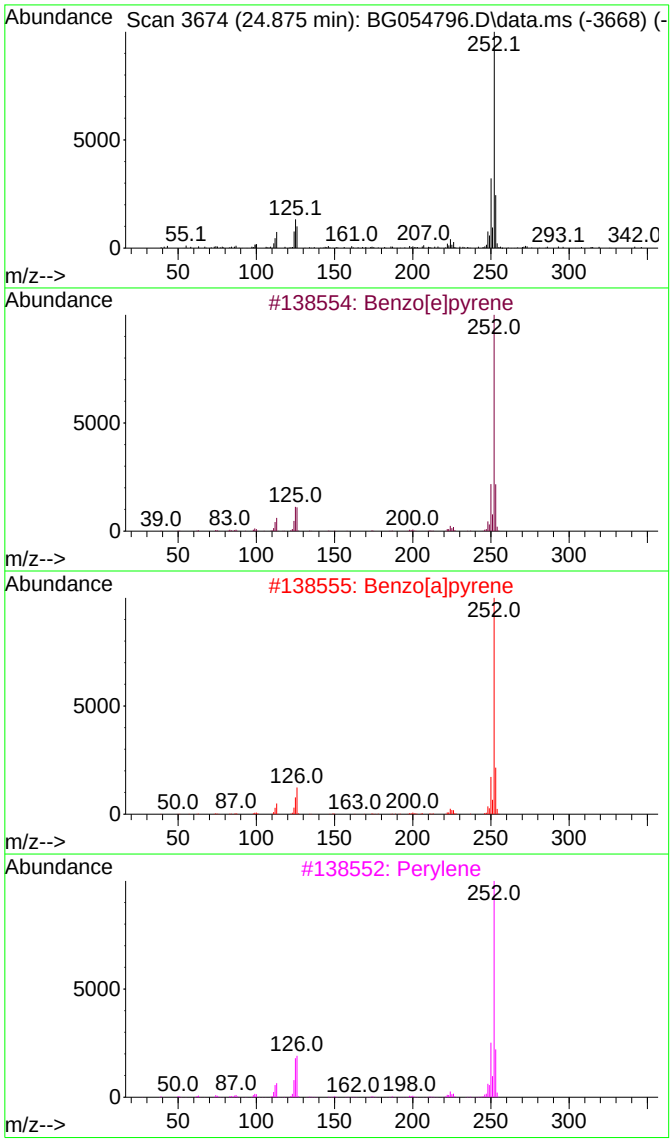
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

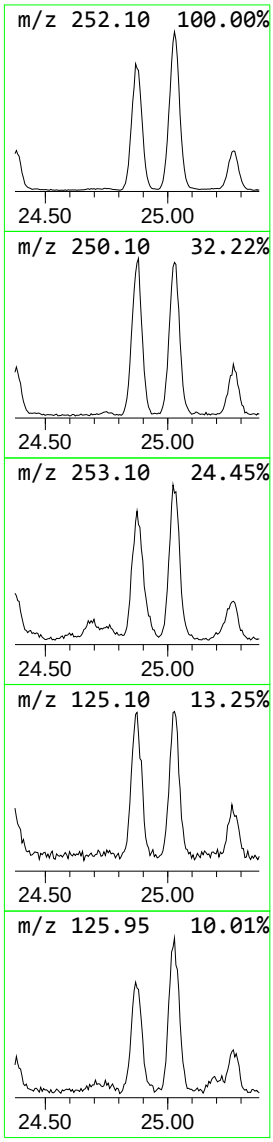
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.875	7.27 ng	285339	Perylene-d12	25.192

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	94
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083022\
Data File : BG054796.D
Acq On : 30 Aug 2022 19:26
Operator : CG/JU
Sample : N4397-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-216

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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-...	5.215	7.1	ng	110951	1	8.153	312018	20.0
Anthracene, 2-m...	18.400	2.4	ng	88576	4	17.530	744059	20.0
Anthracene, 9-m...	18.447	2.9	ng	106336	4	17.530	744059	20.0
4H-Cyclopenta[d...	18.600	4.5	ng	168459	4	17.530	744059	20.0
unknown20.239	20.239	2.6	ng	165952	5	21.820	1258530	20.0
Pyrene, 1-methyl-	20.421	2.2	ng	136866	5	21.820	1258530	20.0
3-Eicosene, (E)-	21.432	4.3	ng	270572	5	21.820	1258530	20.0
Benzo[e]pyrene	24.875	7.3	ng	285339	6	25.192	785110	20.0