LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

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-BG010824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.024	322	329	337	rBV	48975	78464	1.14%	0.142%
2	5.494	402	409	428	rBV	1440490	2341836	33.91%	4.225%
3	7.086	673	680	697	rBV	1312305	2303712	33.36%	4.156%
4	7.920	815	822	830	rBV	461884	789092	11.43%	1.424%
5	9.083	1012	1020	1029	rBV	955736	1717743	24.87%	3.099%
6	10.723	1290	1299	1314	rBV	662250	1214918	17.59%	2.192%
7	13.179	1709	1717	1729	rBV	2990404	4641615	67.22%	8.373%
8	14.559	1943	1952	1959	rBV	1240788	1909356	27.65%	3.444%
9	14.624	1959	1963	1970	rVB2	78997	129401	1.87%	0.233%
10	15.605	2125	2130	2136	rBV	53842	93251	1.35%	0.168%
11	16.052	2198	2206	2224	rBV	2441090	3853758	55.81%	6.952%
12	17.056	2370	2377	2382	rBV9	32307	73481	1.06%	0.133%
13	17.127	2384	2389	2393	rBV	42724	71565	1.04%	0.129%
14	17.309	2414	2420	2424	rBV	1618627	2467001	35.72%	4.450%
15	17.350	2424	2427	2436	rVV	970179	1405852	20.36%	2.536%
16	17.438	2436	2442	2449	rVB	175574	313972	4.55%	0.566%
17	17.715	2483	2489	2494	rBV	87576	163264	2.36%	0.295%
18	18.196	2564	2571	2574	rBV3	240210	403399	5.84%	0.728%
19	18.232	2574	2577	2587	rVV	153692	285493	4.13%	0.515%
20	18.314	2587	2591	2596	rVV2	49464	86169	1.25%	0.155%
21	18.384	2596	2603	2607	rVV3	180316	341046	4.94%	0.615%
22	18.414	2607	2608	2615	rVB	73847	81338	1.18%	0.147%
23	18.684	2649	2654	2658	rBV	90260	123702	1.79%	0.223%
24	18.725	2658	2661	2667	rVB	76459	103106	1.49%	0.186%
25	19.107	2721	2726	2730	rBV6	45148	80116	1.16%	0.145%
26	19.236	2745	2748	2758	rVB3	61031	121544	1.76%	0.219%
27	19.366	2764	2770	2776	rBV	1926521	2590182	37.51%	4.673%
28	19.606	2809	2811	2818	rVB2	57887	84575	1.22%	0.153%
29	19.695	2821	2826	2828	rBV	286721	423563	6.13%	0.764%
30	19.730	2828	2832	2839	rVV	1611166	2301785	33.33%	4.152%
31	19.794	2840	2843	2848	rVB2	69041	110216	1.60%	0.199%
32	19.930	2858	2866	2871	rBV	5207178	6905606	100.00%	12.458%
33	20.047	2881	2886	2893	rBV4	94598	248878	3.60%	0.449%
34	20.188	2906	2910	2911	rBV4	54853	75587	1.09%	0.136%
35	20.223	2912	2916	2924	rVB	238560	351170	5.09%	0.634%
36	20.323	2929	2933	2937	rBV	133862	182906	2.65%	0.330%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

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-BG010824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.382	2940	2943	2946	rVB	93369	120176	1.74%	0.217%
38	20.523	2963	2967	2970	rBV2	68386	92728	1.34%	0.167%
39	20.564	2971	2974	2978	rVV2	57769	85022	1.23%	0.153%
40	20.975	3041	3044	3049	rVB2	106792	157493	2.28%	0.284%
41	21.158	3070	3075	3079	rBV2	108086	187845	2.72%	0.339%
42	21.210	3079	3084	3087	rBV4	176207	319319	4.62%	0.576%
43	21.304	3097	3100	3110	rVB2	107207	198605	2.88%	0.358%
44	21.457	3121	3126	3131	rVB	589541	819194	11.86%	1.478%
45	21.569	3137	3145	3150	rBV2	1851517	4107908	59.49%	7.411%
46	21.616	3150	3153	3164	rVB	657330	1098860	15.91%	1.982%
47	21.763	3174	3178	3187	rVB3	161396	370323	5.36%	0.668%
48	22.292	3264	3268	3272	rVB2	67982	109045	1.58%	0.197%
49	22.350	3273	3278	3283	rVB3	210462	356372	5.16%	0.643%
50	23.208	3420	3424	3431	rVB	200587	366310	5.30%	0.661%
51	23.361	3448	3450	3459	rVB5	88159	179715	2.60%	0.324%
52	23.731	3505	3513	3520	rBV2	483462	1572231	22.77%	2.836%
53	23.802	3522	3525	3534	rVB3	406385	826875	11.97%	1.492%
54	24.442	3627	3634	3646	rVB2	310487	897302	12.99%	1.619%
55	24.583	3650	3658	3668	rVB	421673	1138420	16.49%	2.054%
56	24.736	3675	3684	3693	rBV	1026137	2879169	41.69%	5.194%
57	25.247	3766	3771	3779	rVB6	204500	503426	7.29%	0.908%
58	27.944	4222	4230	4243	rVB5	153888	577683	8.37%	1.042%

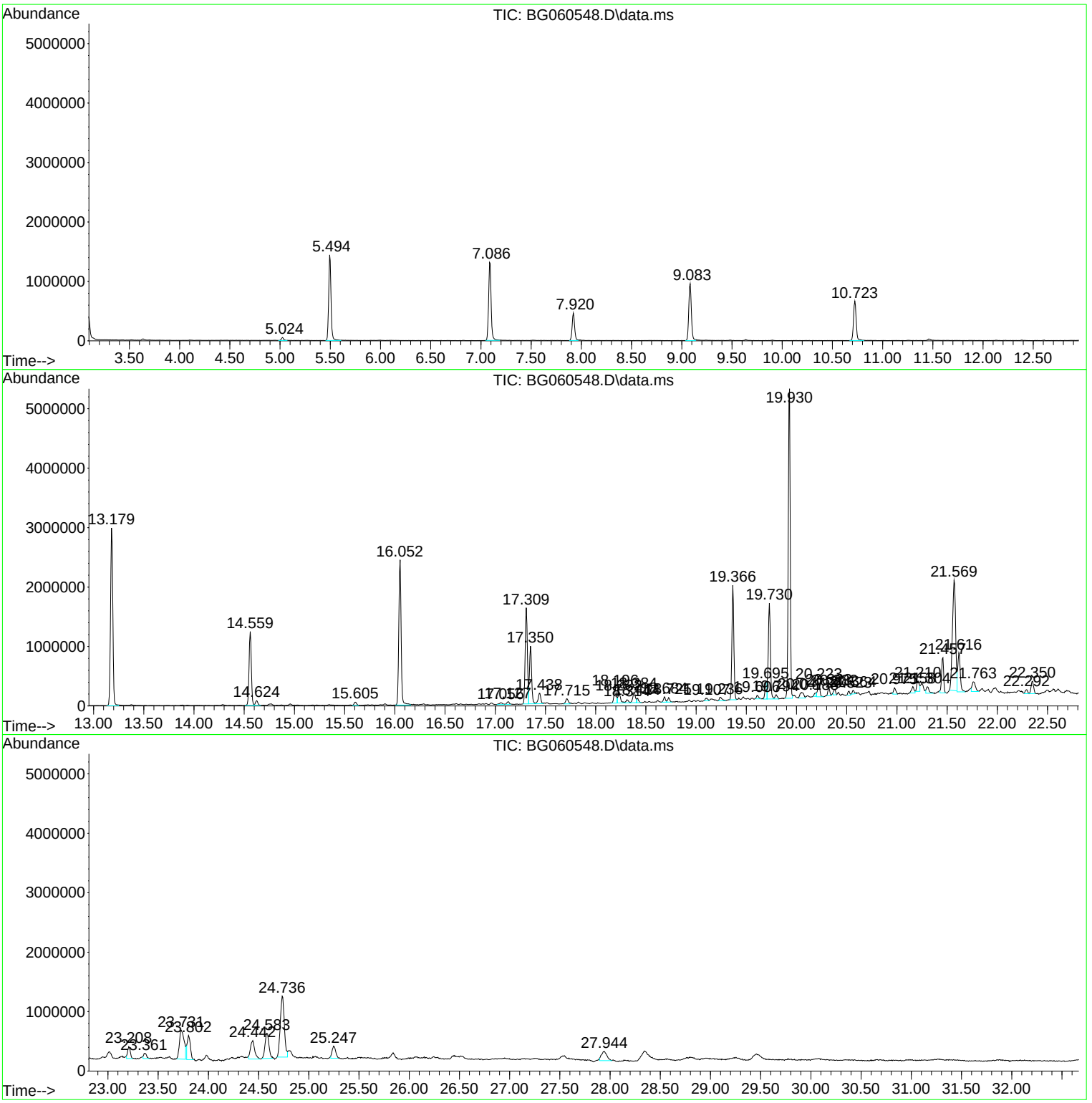
Sum of corrected areas: 55432683

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

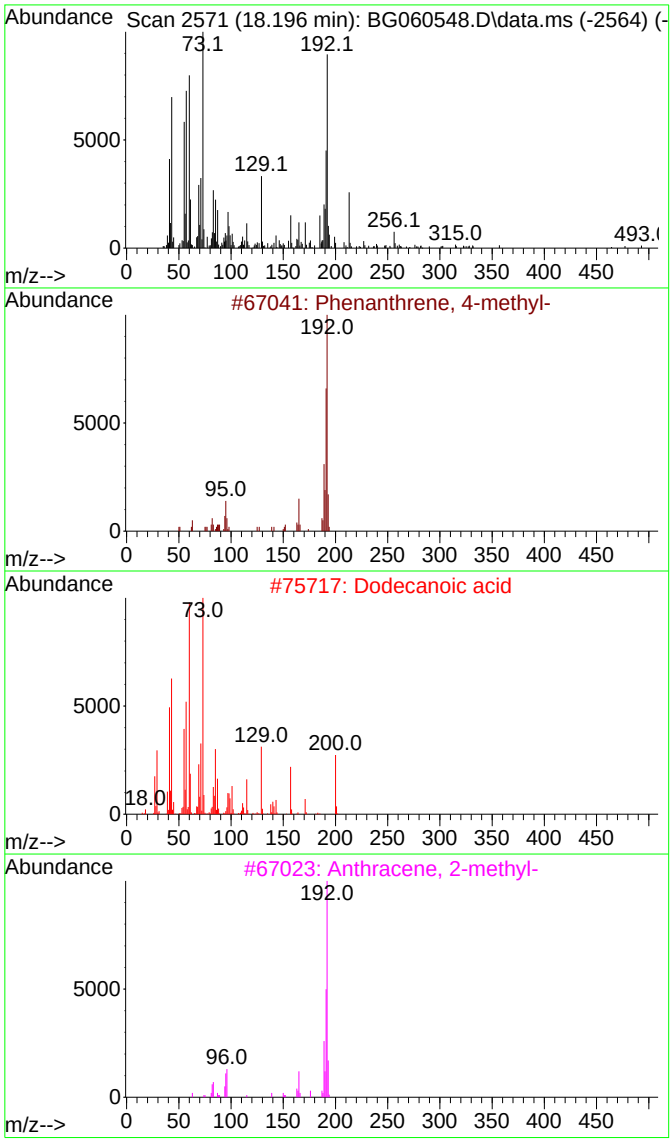
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

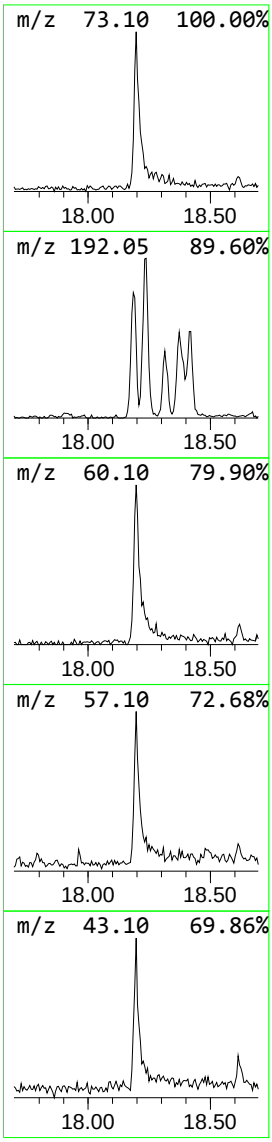
****

Peak Number 1 Phenanthrene, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.196	3.27 ng	403399	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70
2	Dodecanoic acid	200	C12H24O2	000143-07-7	46
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	43
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

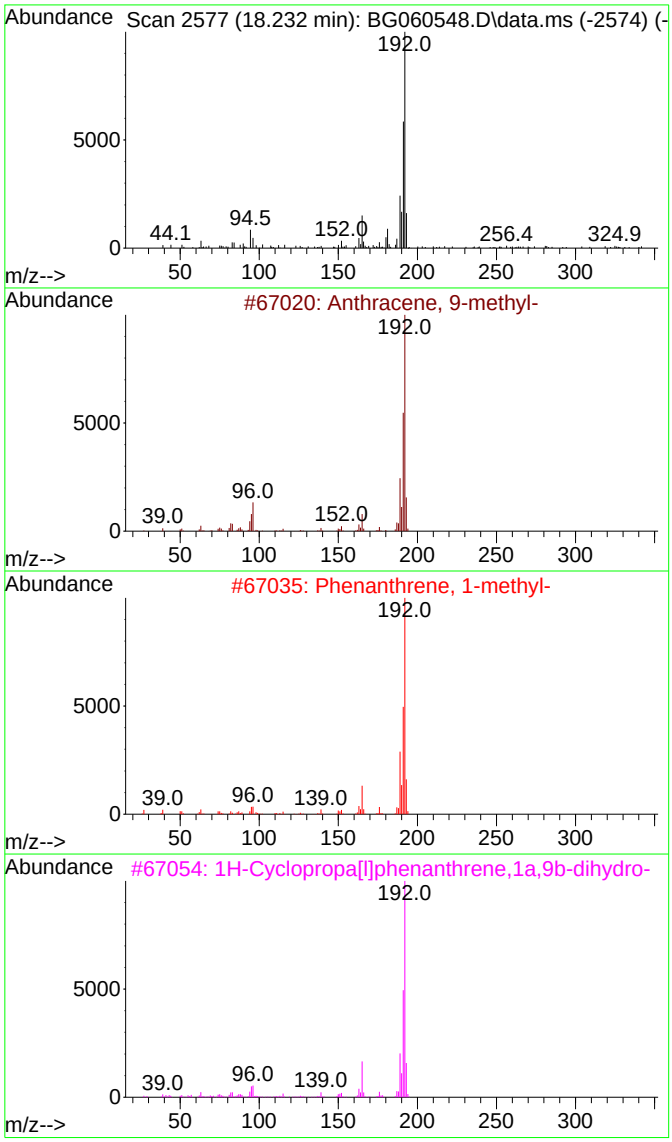
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

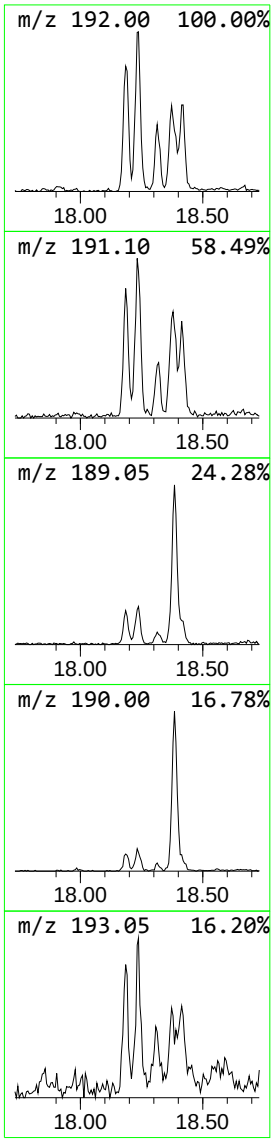
****

Peak Number 2 Anthracene, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	2.31 ng	285493	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	87
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

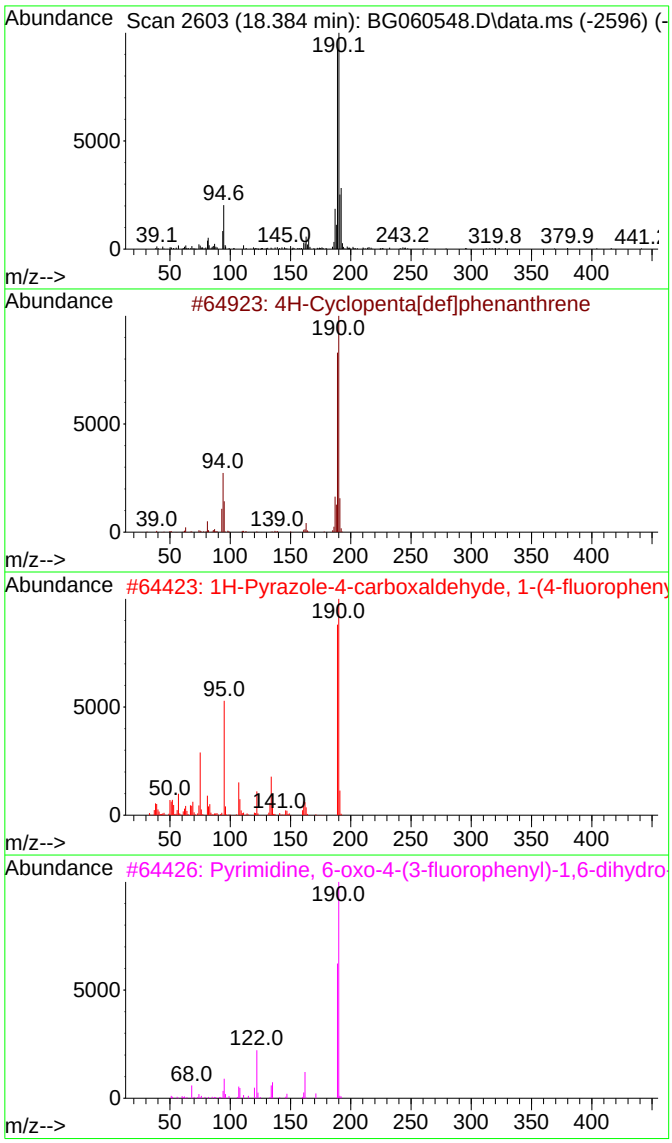
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

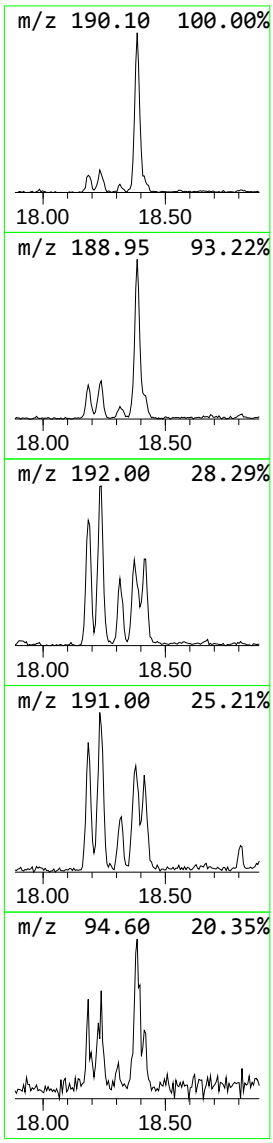
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.384	2.76 ng	341046	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	52
3	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	1-Aminocyclopentanecarboxylic ac...	375	C19H34ClNO4	1000329-17-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

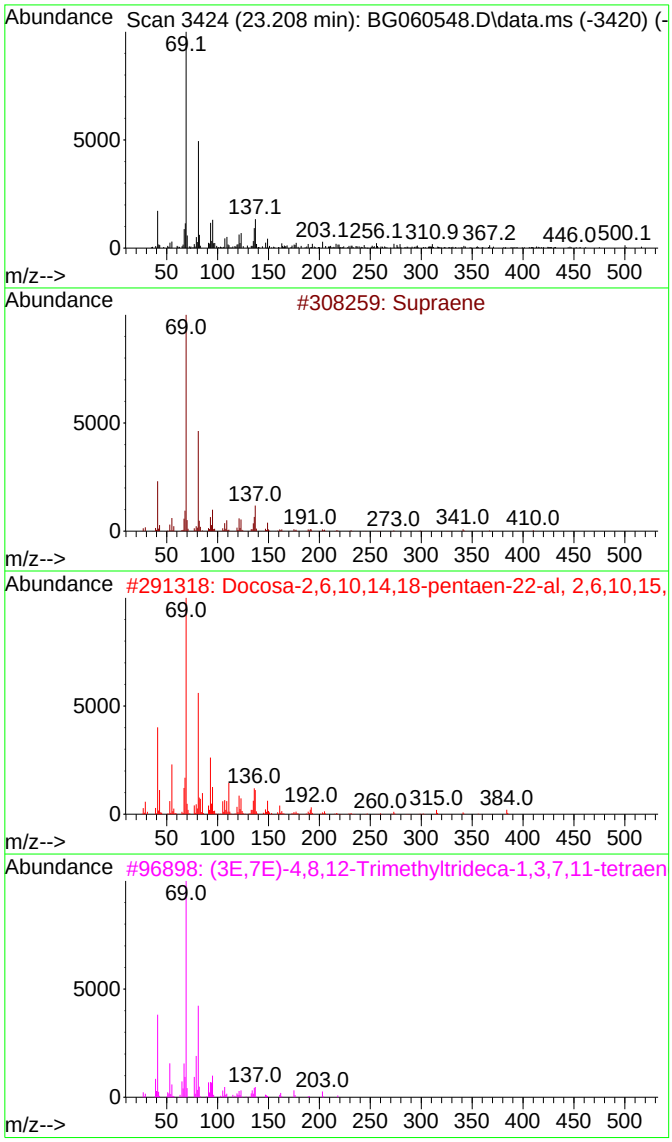
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

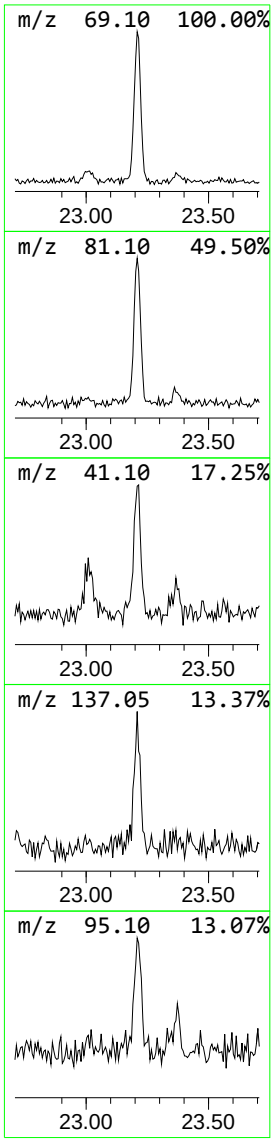
****

Peak Number 4 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.208	2.54 ng	366310	Perylene-d12	24.736

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	98
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
3	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72
4	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	72
5	Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

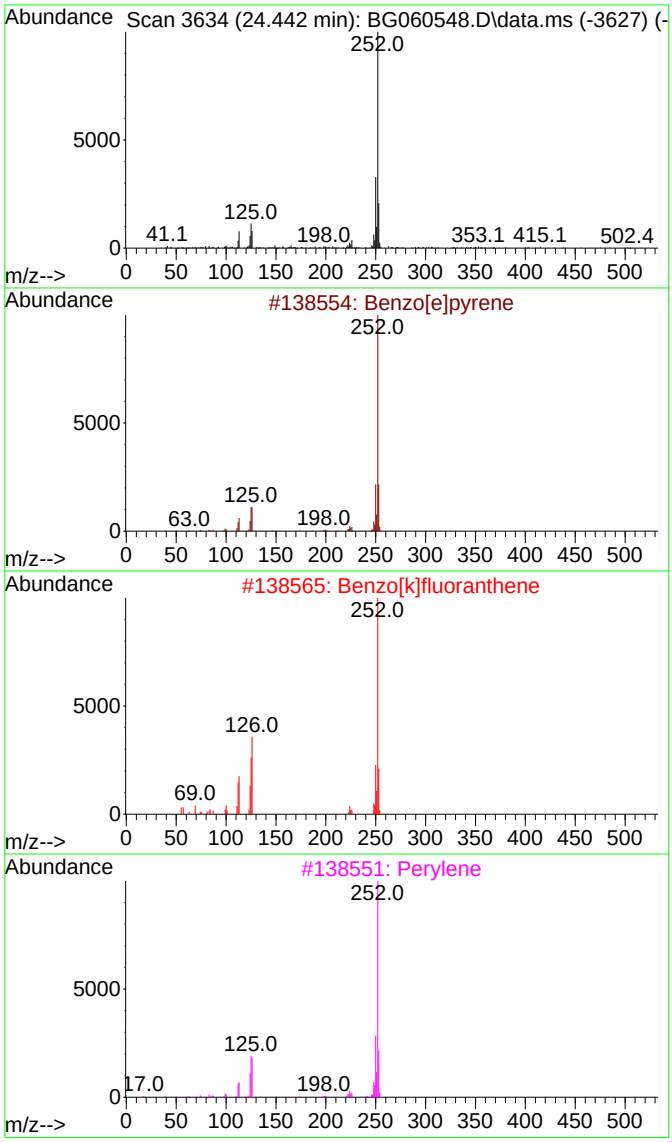
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

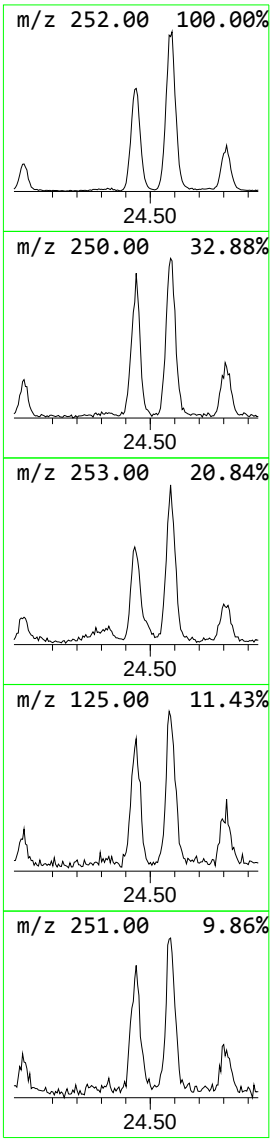
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.442	6.23 ng	897302	Perylene-d12	24.736

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

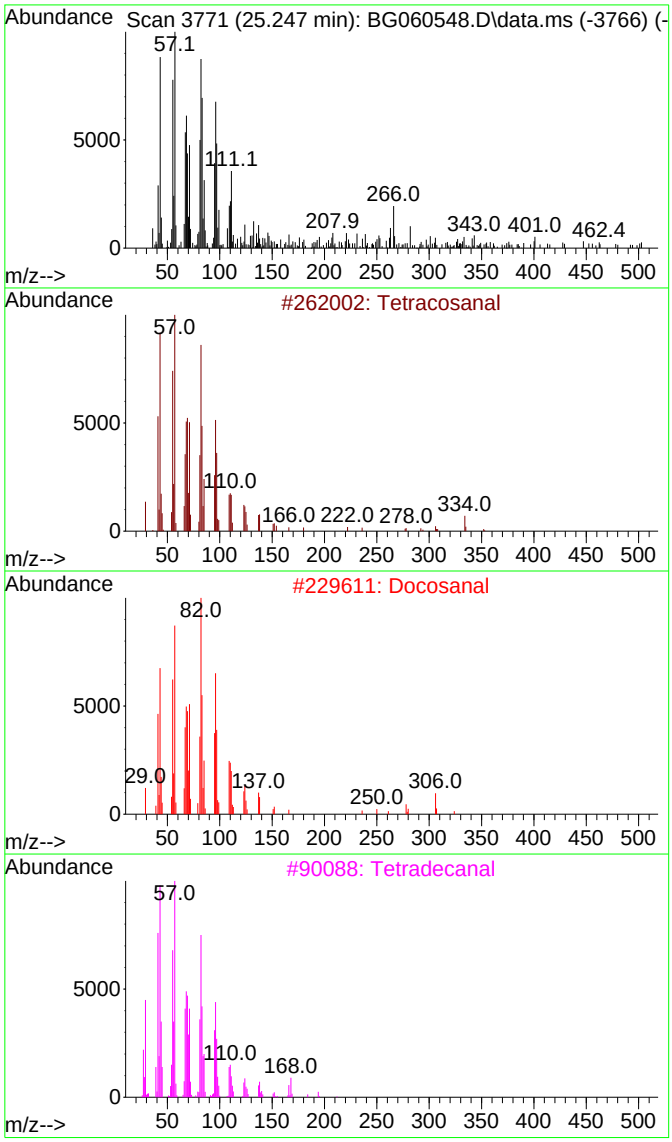
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

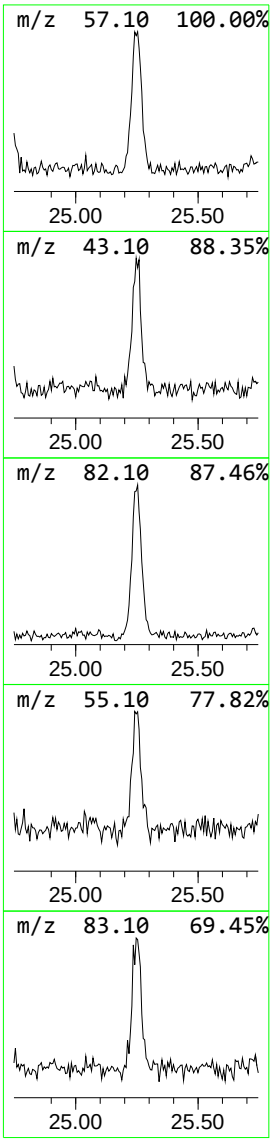
****

Peak Number 6 Tetracosanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.247	3.50 ng	503426	Perylene-d12	24.736

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosanal	352	C24H48O	057866-08-7	93
2	Docosanal	324	C22H44O	057402-36-5	86
3	Tetradecanal	212	C14H28O	000124-25-4	86
4	Eicosanal-	296	C20H40O	002400-66-0	81
5	Octadecanal	268	C18H36O	000638-66-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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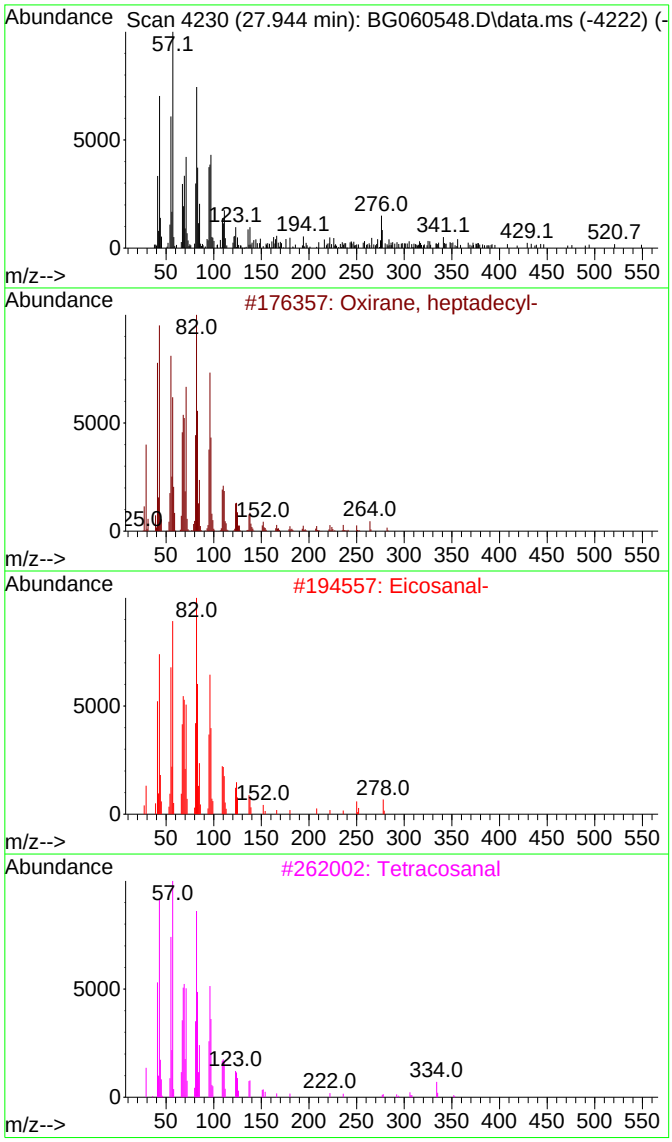
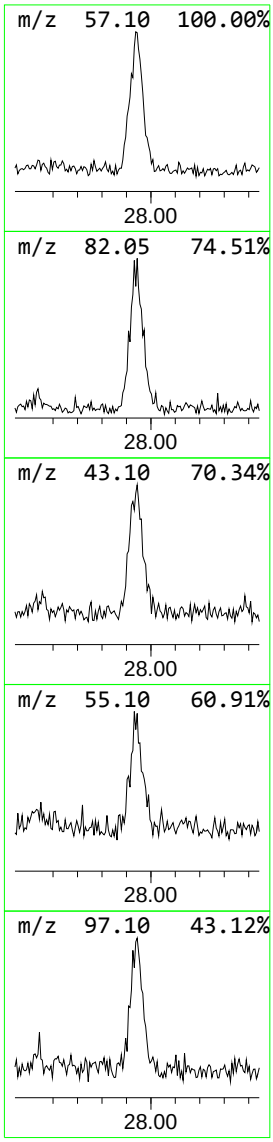
Peak Number 7 Oxirane, heptadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.944	4.01 ng	577683	Perylene-d12	24.736

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
2	Eicosanal-	296	C20H40O	002400-66-0	80
3	Tetracosanal	352	C24H48O	057866-08-7	74
4	Hexacosanal	380	C26H52O	026627-85-0	72
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020224\
Data File : BG060548.D
Acq On : 2 Feb 2024 1:04
Operator : MA/JU
Sample : P1313-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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
Phenanthrene, 4...	18.196	3.3	ng	403399	4	17.309	2467000	20.0
Anthracene, 9-m...	18.232	2.3	ng	285493	4	17.309	2467000	20.0
4H-Cyclopenta[d...	18.384	2.8	ng	341046	4	17.309	2467000	20.0
Supraene	23.208	2.5	ng	366310	6	24.736	2879170	20.0
Benzo[e]pyrene	24.442	6.2	ng	897302	6	24.736	2879170	20.0
Tetracosanal	25.247	3.5	ng	503426	6	24.736	2879170	20.0
Oxirane, heptad...	27.944	4.0	ng	577683	6	24.736	2879170	20.0