LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

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-BM092024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	312	317	323	rVB	78282	108053	1.12%	0.118%
2	5.410	388	395	405	rBV	1210725	1805268	18.70%	1.968%
3	6.998	657	665	673	rBV	1214643	1890355	19.58%	2.061%
4	7.839	798	808	815	rBV	1714508	2667909	27.63%	2.909%
5	8.986	994	1003	1010	rBV	694703	1130232	11.71%	1.232%
6	10.633	1274	1283	1289	rBV	2118203	3624577	37.54%	3.952%
7	13.092	1693	1701	1710	rBV	1579764	2288145	23.70%	2.495%
8	14.468	1927	1935	1941	rBV	2910894	4101828	42.48%	4.473%
9	14.533	1941	1946	1953	rVB	218759	342587	3.55%	0.374%
10	14.868	1997	2003	2008	rVB	149654	242698	2.51%	0.265%
11	15.510	2106	2112	2118	rBV	276800	414209	4.29%	0.452%
12	15.815	2158	2164	2172	rVB3	207907	373405	3.87%	0.407%
13	15.951	2181	2187	2196	rBV2	1016535	1530804	15.85%	1.669%
14	16.515	2277	2283	2288	rBV2	64913	107974	1.12%	0.118%
15	16.745	2315	2322	2325	rBV3	57763	102508	1.06%	0.112%
16	16.856	2337	2341	2350	rVB4	76775	130802	1.35%	0.143%
17	16.939	2350	2355	2360	rBV2	72908	149547	1.55%	0.163%
18	17.021	2365	2369	2380	rVB	155240	264967	2.74%	0.289%
19	17.204	2394	2400	2404	rBV	3027192	4404733	45.62%	4.803%
20	17.245	2404	2407	2413	rVV	2843460	3752245	38.86%	4.091%
21	17.333	2417	2422	2428	rVV	893395	1320320	13.67%	1.440%
22	17.392	2428	2432	2438	rVB3	60901	107734	1.12%	0.117%
23	17.603	2463	2468	2471	rBV	100192	137977	1.43%	0.150%
24	17.721	2484	2488	2492	rVB2	84924	108256	1.12%	0.118%
25	18.080	2544	2549	2553	rBV	321705	640121	6.63%	0.698%
26	18.127	2553	2557	2564	rVB	464311	712803	7.38%	0.777%
27	18.203	2565	2570	2575	rBV2	231044	348763	3.61%	0.380%
28	18.274	2576	2582	2586	rVV3	582159	1071289	11.09%	1.168%
29	18.309	2586	2588	2594	rVB	222485	258782	2.68%	0.282%
30	18.574	2629	2633	2637	rBV	254784	359787	3.73%	0.392%
31	18.609	2637	2639	2647	rVB2	127119	178411	1.85%	0.195%
32	18.821	2672	2675	2680	rVB2	74408	96919	1.00%	0.106%
33	18.874	2680	2684	2687	rVV	98911	121235	1.26%	0.132%
34	18.909	2687	2690	2694	rVB2	81052	108712	1.13%	0.119%
35	18.992	2700	2704	2709	rBV	206961	326159	3.38%	0.356%
36	19.056	2709	2715	2718	rVV4	128106	231948	2.40%	0.253%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

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-BM092024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.133	2723	2728	2735	rBV	217496	370115	3.83%	0.404%
38	19.256	2743	2749	2755	rBV	7146834	8939397	92.58%	9.747%
39	19.497	2786	2790	2794	rBV	180297	223123	2.31%	0.243%
40	19.586	2800	2805	2806	rBV	1007642	1177832	12.20%	1.284%
41	19.615	2806	2810	2818	rVV	5387277	7376589	76.39%	8.043%
42	19.686	2819	2822	2829	rVB2	216771	361153	3.74%	0.394%
43	19.815	2836	2844	2849	rBV2	2128169	3031353	31.39%	3.305%
44	19.933	2859	2864	2866	rBV	295029	504258	5.22%	0.550%
45	20.074	2884	2888	2890	rBV3	183152	296794	3.07%	0.324%
46	20.109	2890	2894	2898	rVB	641576	869480	9.00%	0.948%
47	20.209	2907	2911	2914	rBV	460161	559441	5.79%	0.610%
48	20.268	2915	2921	2924	rVV2	401891	677992	7.02%	0.739%
49	20.303	2925	2927	2931	rVB	143306	157427	1.63%	0.172%
50	20.403	2941	2944	2948	rBV	175267	235204	2.44%	0.256%
51	20.450	2949	2952	2956	rVB2	180245	239865	2.48%	0.262%
52	20.850	3017	3020	3027	rVB	365399	549276	5.69%	0.599%
53	21.074	3055	3058	3061	rVB	302564	344546	3.57%	0.376%
54	21.115	3061	3065	3070	rVV2	408461	696491	7.21%	0.759%
55	21.168	3071	3074	3082	rVB2	376863	580947	6.02%	0.633%
56	21.421	3110	3117	3123	rBV3	4051931	9655862	100.00%	10.529%
57	21.474	3123	3126	3135	rVB	2352561	3311066	34.29%	3.610%
58	21.615	3147	3150	3157	rBV2	352468	631529	6.54%	0.689%
59	23.503	3463	3471	3478	rBV	1709825	5188819	53.74%	5.658%
60	24.174	3579	3585	3597	rVB	933909	2482034	25.70%	2.706%
61	24.309	3601	3608	3622	rVB	1410303	3504233	36.29%	3.821%
62	24.450	3625	3632	3639	rBV	1669425	4182913	43.32%	4.561%

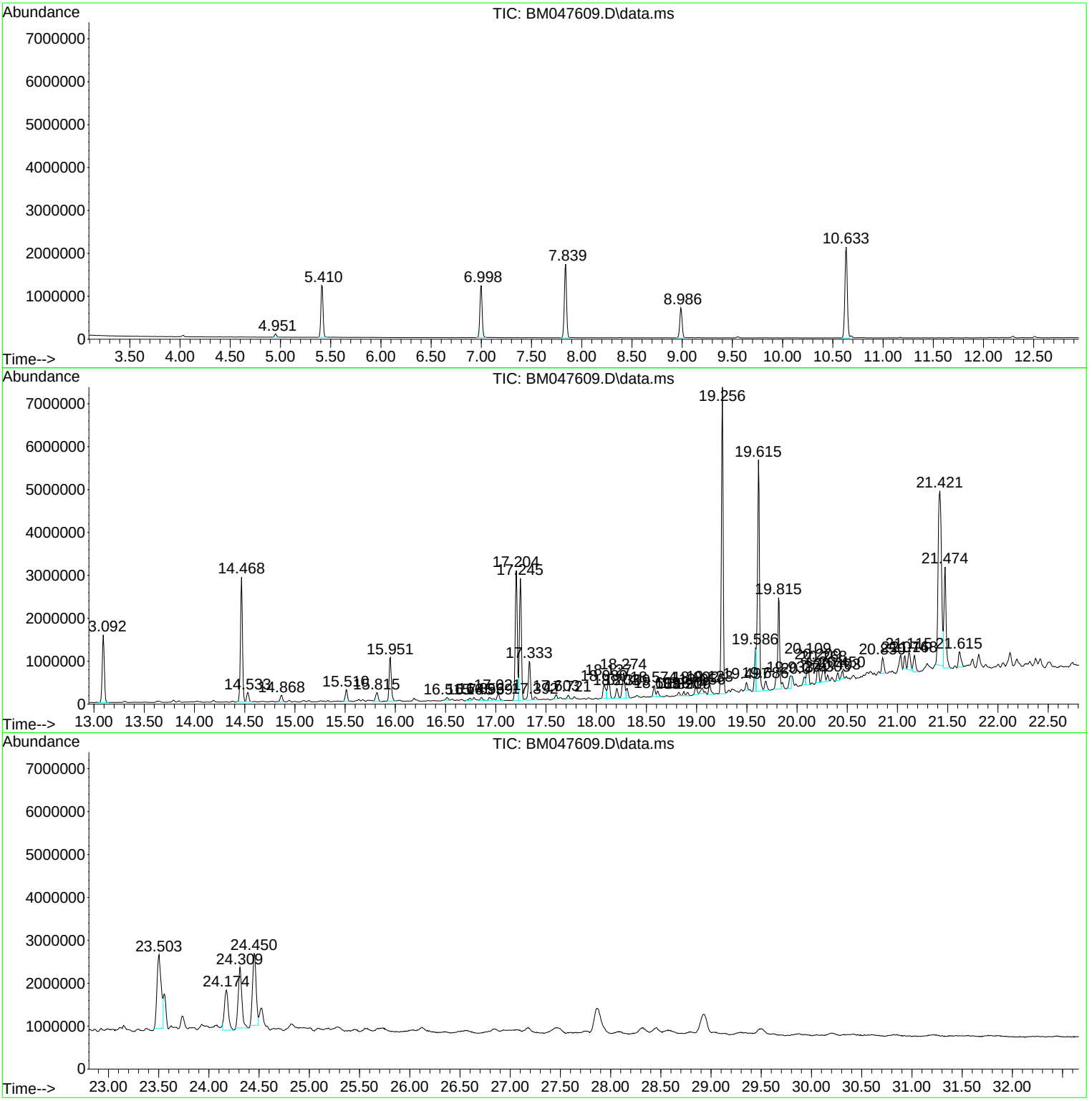
Sum of corrected areas: 91709801

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.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\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

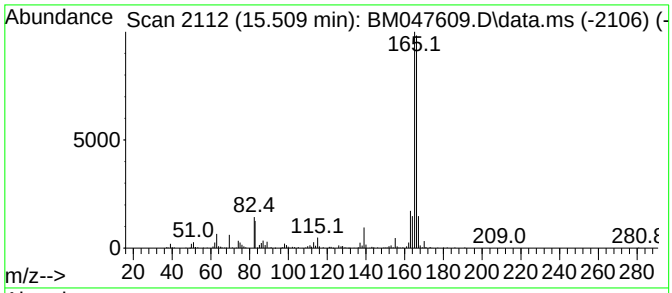
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

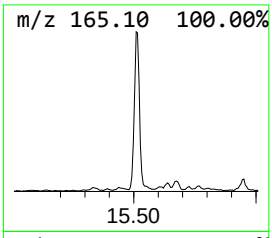
****

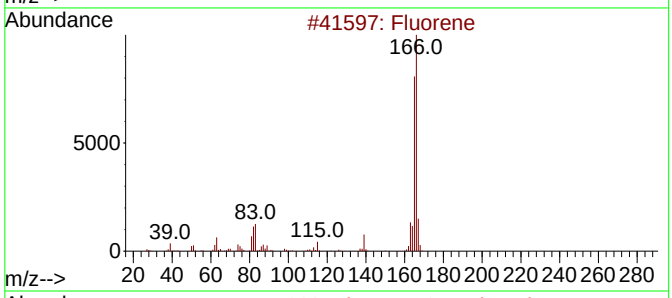
Peak Number 1 Fluorene-9-methanol Concentration Rank 5

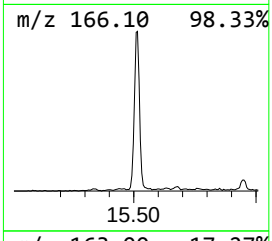
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.509	2.02 ng	414209	Acenaphthene-d10	14.468

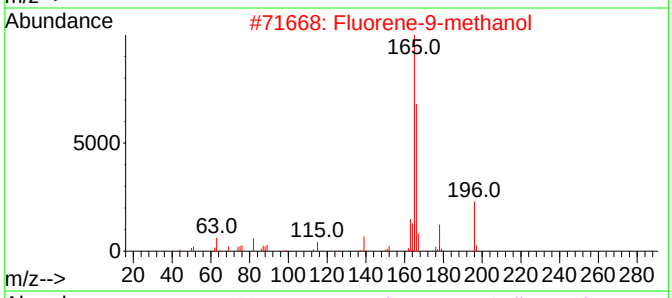
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene	166	C13H10	000086-73-7	96
2	Fluorene-9-methanol	196	C14H12O	024324-17-2	83
3	Benzene, 5-heptene-1,3-diyn-1-yl-	166	C13H10	013678-98-3	56
4	Benzene, 1,1'-(diazomethylene)bis-	194	C13H10N2	000883-40-9	53
5	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	50

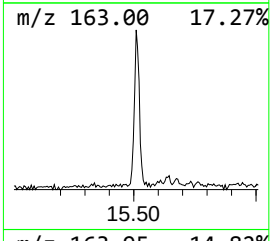


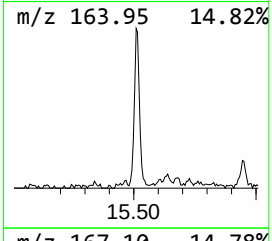


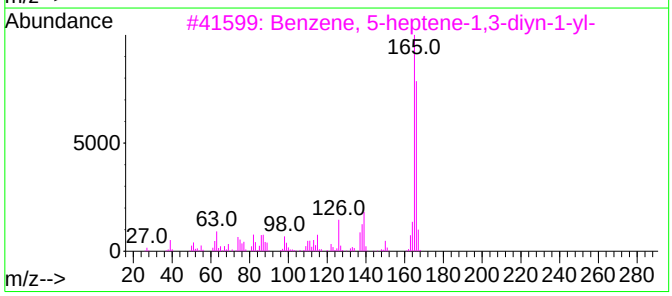


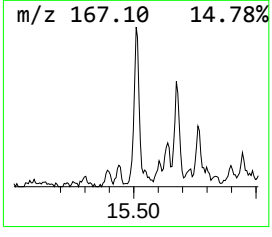












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

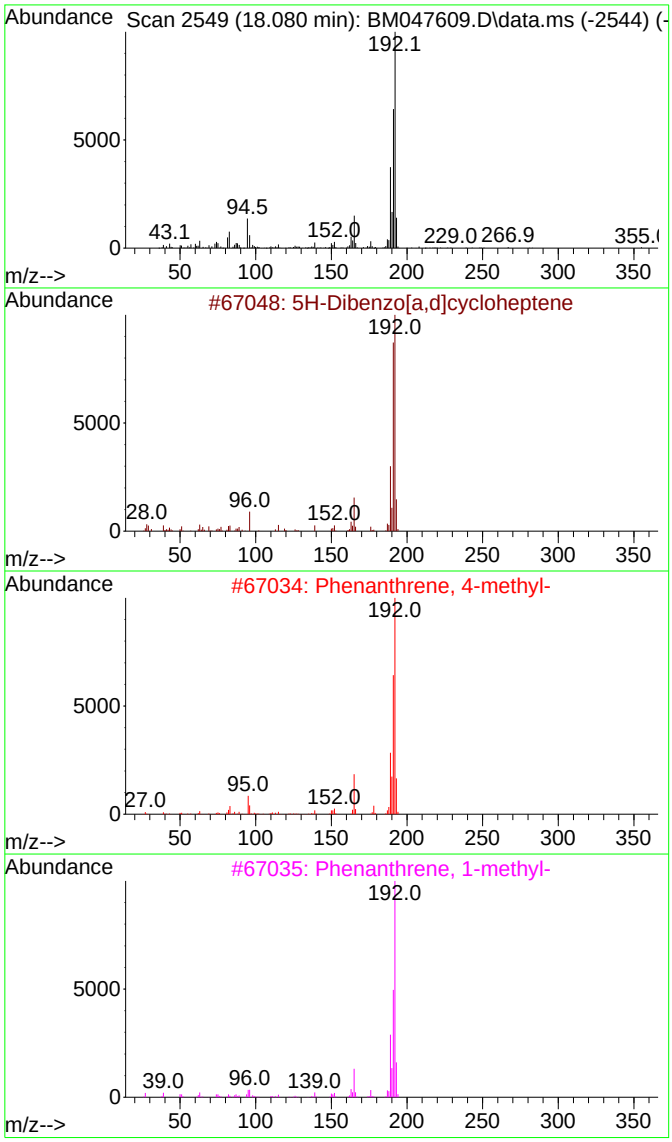
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

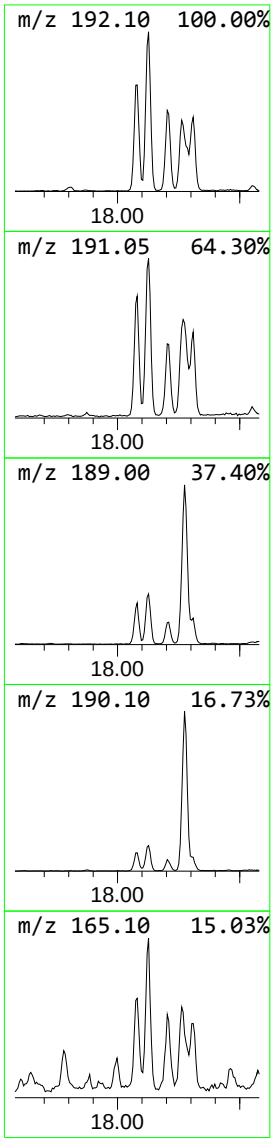
****

Peak Number 2 5H-Dibenzo[a,d]cycloheptene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	2.91 ng	640121	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	95
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

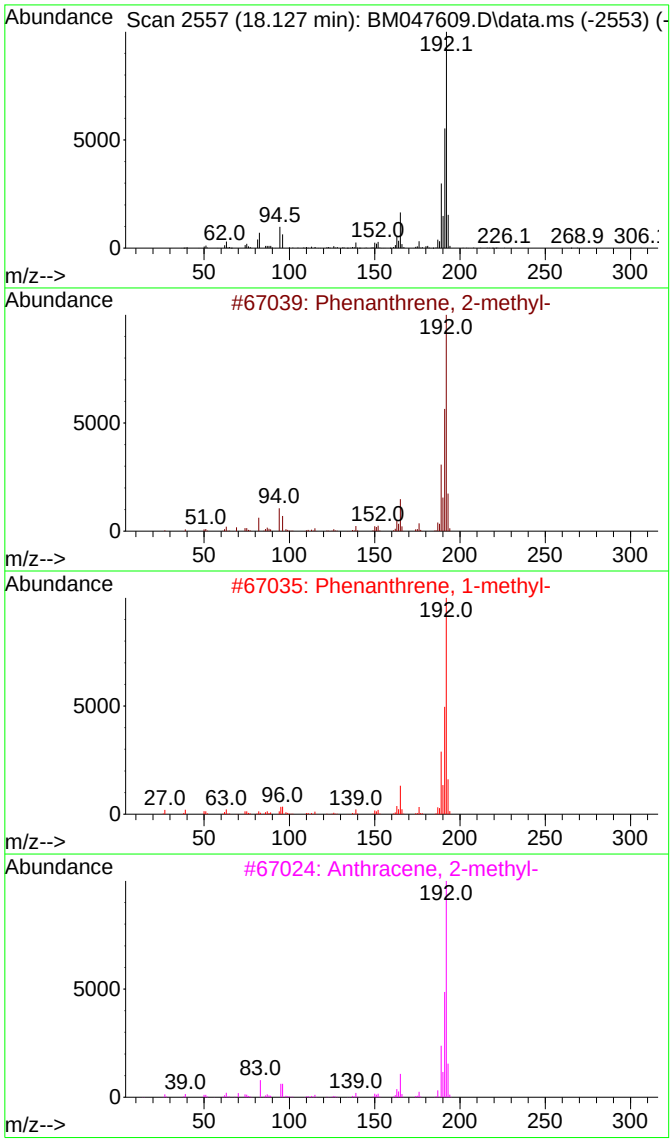
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

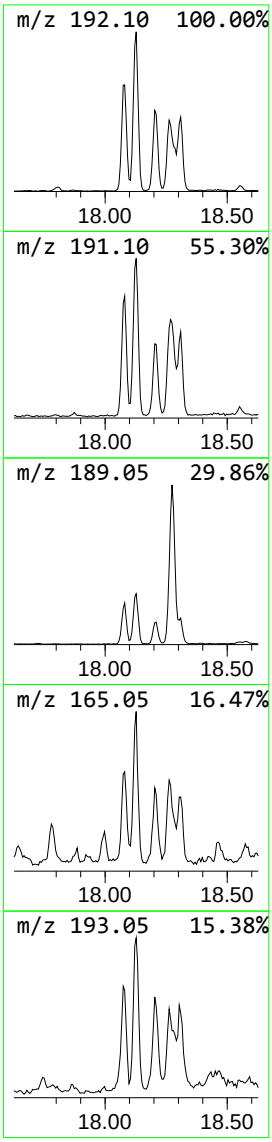
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	3.24 ng	712803	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

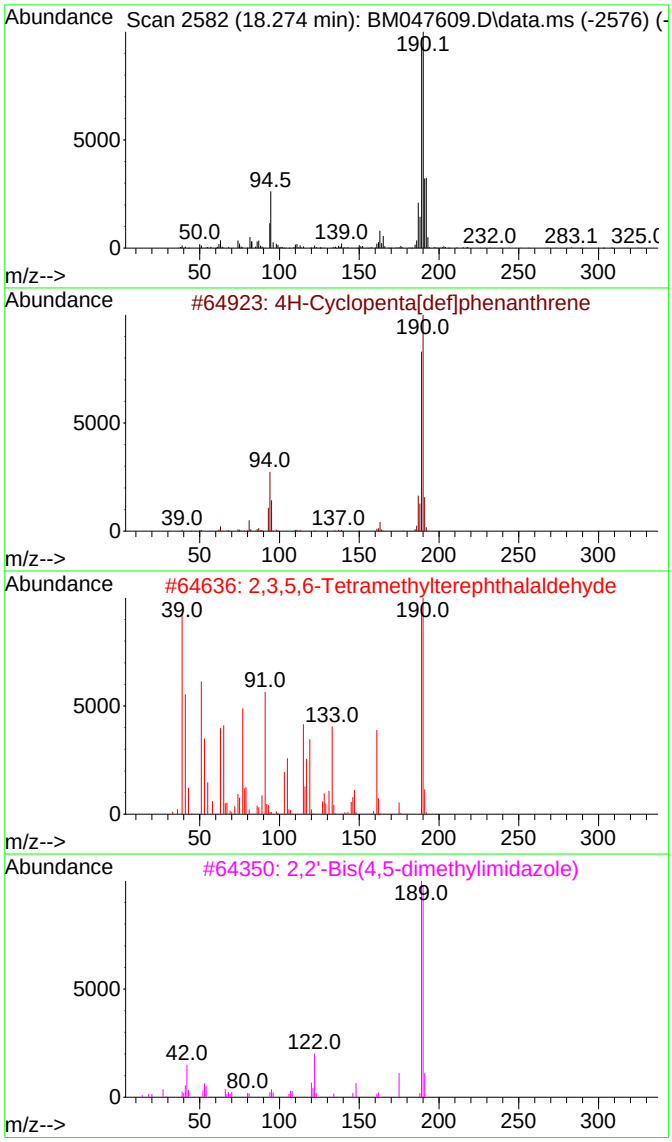
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

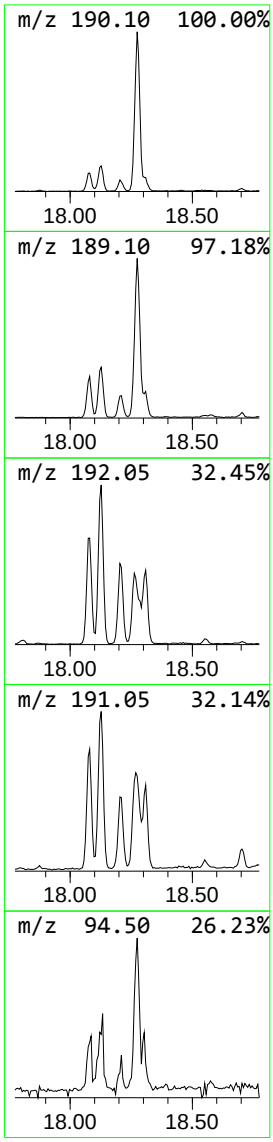
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	4.86 ng	1071290	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
4	1-Aminocyclopentanecarboxylic ac...	375	C19H34ClNO4	1000329-17-1	27
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

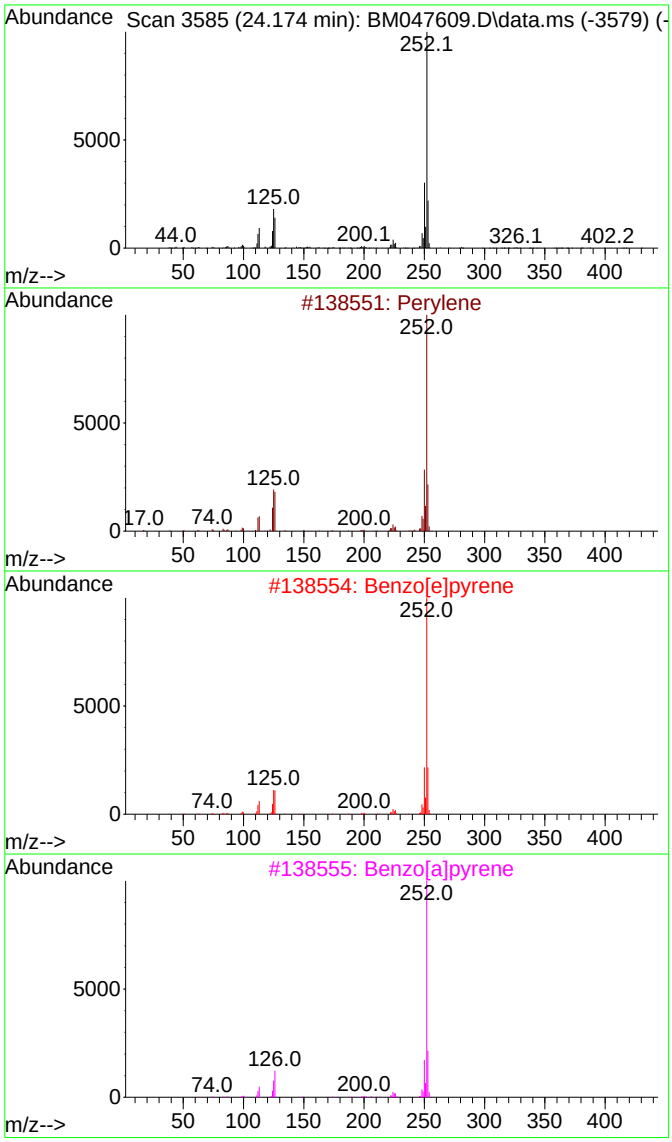
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

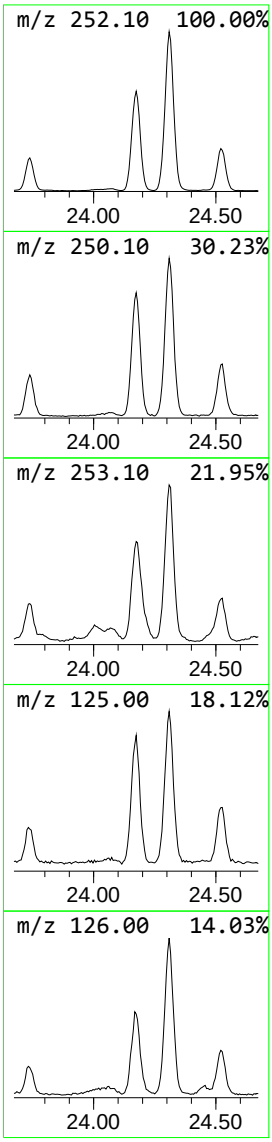
****

Peak Number 5 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.174	11.87 ng	2482030	Perylene-d12	24.456

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047609.D
Acq On : 23 Sep 2024 18:21
Operator : RC/JU
Sample : P4146-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-02-092024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.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
Fluorene-9-meth...	15.509	2.0	ng	414209	3	14.468	4101830	20.0
5H-Dibenzo[a,d]...	18.080	2.9	ng	640121	4	17.203	4404730	20.0
Phenanthrene, 2...	18.127	3.2	ng	712803	4	17.203	4404730	20.0
4H-Cyclopenta[d...	18.274	4.9	ng	1071290	4	17.203	4404730	20.0
Perylene	24.174	11.9	ng	2482030	6	24.456	4182910	20.0