LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055766.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.282	331	339	347	rBV	124259	192894	10.20%	1.514%
2	5.764	414	421	435	rBV	461292	757262	40.05%	5.945%
3	6.898	609	614	622	rVB2	12070	20011	1.06%	0.157%
4	7.380	689	696	711	rBV	500593	875454	46.30%	6.873%
5	7.668	738	745	751	rBV2	18616	29363	1.55%	0.231%
6	8.238	834	842	848	rBV	99239	167763	8.87%	1.317%
7	9.407	1032	1041	1051	rBV	296917	527653	27.91%	4.143%
8	11.064	1316	1323	1330	rBV	156795	277486	14.68%	2.179%
9	13.484	1728	1735	1746	rBV	834264	1256072	66.43%	9.862%
10	14.724	1941	1946	1950	rBV	15536	19754	1.04%	0.155%
11	14.859	1961	1969	1975	rBV	285506	439391	23.24%	3.450%
12	14.918	1975	1979	1987	rVB2	13789	21492	1.14%	0.169%
13	15.253	2026	2036	2043	rVB	14304	26846	1.42%	0.211%
14	15.670	2097	2107	2111	rVB	18788	28275	1.50%	0.222%
15	15.899	2138	2146	2153	rBV3	18966	32027	1.69%	0.251%
16	16.199	2185	2197	2207	rBV2	27248	52542	2.78%	0.413%
17	16.340	2215	2221	2231	rBV	740753	1166763	61.71%	9.161%
18	16.528	2248	2253	2255	rBV2	18896	23948	1.27%	0.188%
19	17.251	2370	2376	2384	rBV	65524	120231	6.36%	0.944%
20	17.321	2384	2388	2392	rVV2	21325	27348	1.45%	0.215%
21	17.603	2426	2436	2439	rBV	348346	553528	29.28%	4.346%
22	17.644	2439	2443	2449	rVB	167308	253376	13.40%	1.989%
23	17.732	2449	2458	2462	rBV	42938	71210	3.77%	0.559%
24	17.997	2497	2503	2510	rBV2	14966	33297	1.76%	0.261%
25	18.061	2510	2514	2519	rVB	17786	23719	1.25%	0.186%
26	18.461	2577	2582	2588	rBV3	58949	114069	6.03%	0.896%
27	18.520	2588	2592	2597	rVV	42715	65191	3.45%	0.512%
28	18.602	2601	2606	2610	rVV	17972	25492	1.35%	0.200%
29	18.667	2611	2617	2621	rVV3	31446	62918	3.33%	0.494%
30	18.702	2621	2623	2627	rVB2	19974	21976	1.16%	0.173%
31	18.743	2627	2630	2637	rBV2	15095	23146	1.22%	0.182%
32	18.872	2649	2652	2657	rVB3	18738	22552	1.19%	0.177%
33	18.960	2662	2667	2671	rBV	20921	26843	1.42%	0.211%
34	19.002	2671	2674	2681	rVB2	13171	20695	1.09%	0.162%
35	19.372	2732	2737	2742	rBV	28987	48530	2.57%	0.381%
36	19.513	2756	2761	2770	rBV5	17088	31433	1.66%	0.247%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.642	2777	2783	2789	rVB	229943	328542	17.38%	2.579%
38	19.724	2793	2797	2804	rVB6	21209	36344	1.92%	0.285%
39	19.965	2831	2838	2840	rBV3	50826	85797	4.54%	0.674%
40	20.000	2840	2844	2851	rVV	212034	304801	16.12%	2.393%
41	20.065	2851	2855	2860	rVB	20344	29113	1.54%	0.229%
42	20.188	2869	2876	2881	rBV	1444717	1890738	100.00%	14.845%
43	20.312	2893	2897	2899	rBV2	20386	32083	1.70%	0.252%
44	20.482	2916	2926	2933	rBV4	34872	92256	4.88%	0.724%
45	20.588	2940	2944	2947	rBV	14800	21326	1.13%	0.167%
46	20.647	2947	2954	2957	rVV2	29047	58419	3.09%	0.459%
47	20.788	2974	2978	2981	rBV	18940	27767	1.47%	0.218%
48	20.829	2983	2985	2992	rVB	15181	24884	1.32%	0.195%
49	21.264	3055	3059	3065	rVB	30548	46871	2.48%	0.368%
50	21.499	3095	3099	3103	rBV2	29151	49440	2.61%	0.388%
51	21.745	3138	3141	3148	rVB	28162	40011	2.12%	0.314%
52	21.892	3157	3166	3171	rBV3	370889	854612	45.20%	6.710%
53	21.945	3171	3175	3187	rVB	109378	210139	11.11%	1.650%
54	24.207	3553	3560	3567	rBV	65218	214398	11.34%	1.683%
55	24.971	3686	3690	3699	rVB	39114	98878	5.23%	0.776%
56	25.124	3710	3716	3725	rVB	52375	145083	7.67%	1.139%
57	25.294	3734	3745	3754	rBV2	220768	684832	36.22%	5.377%

Sum of corrected areas: 12736884

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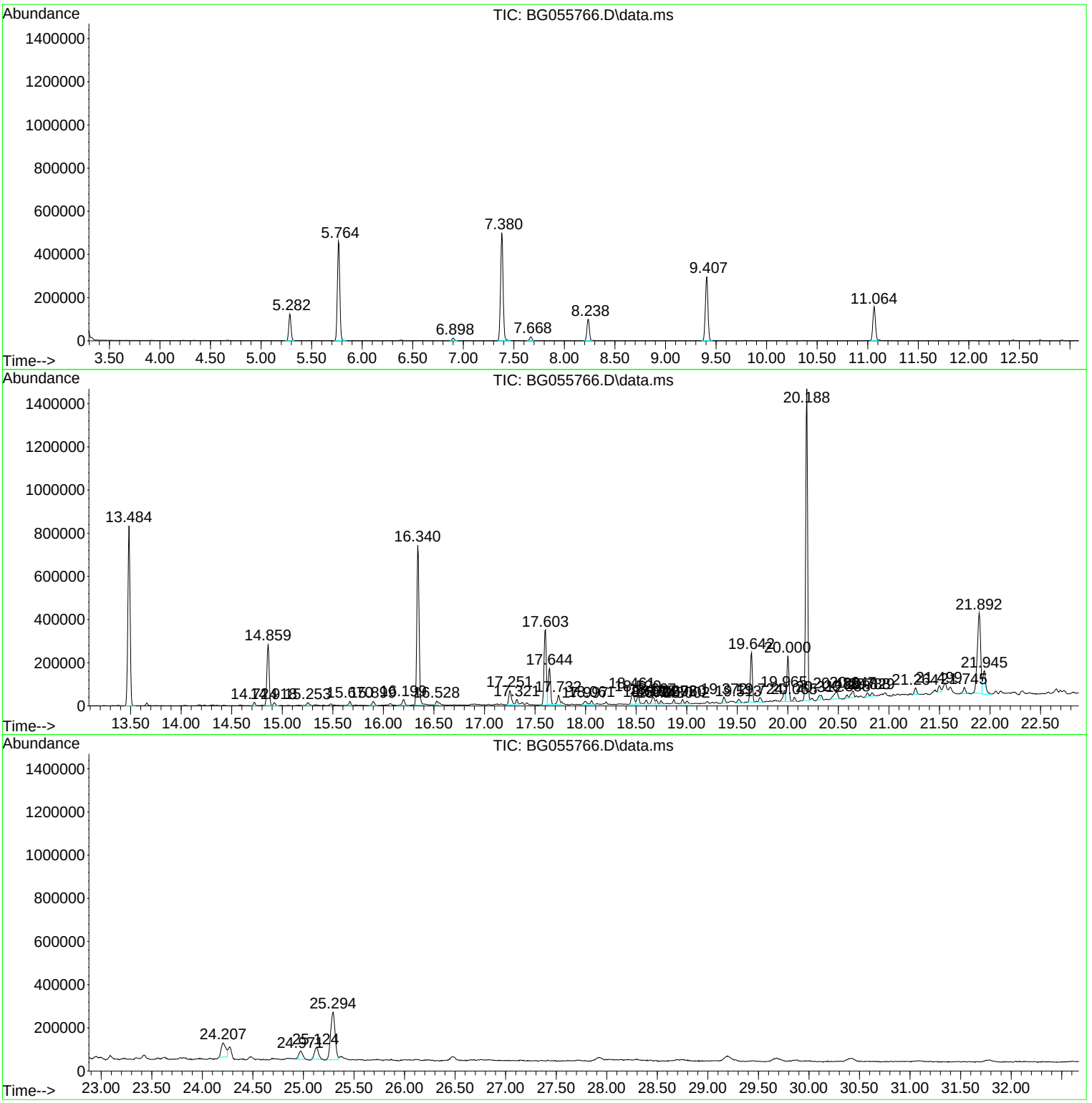
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
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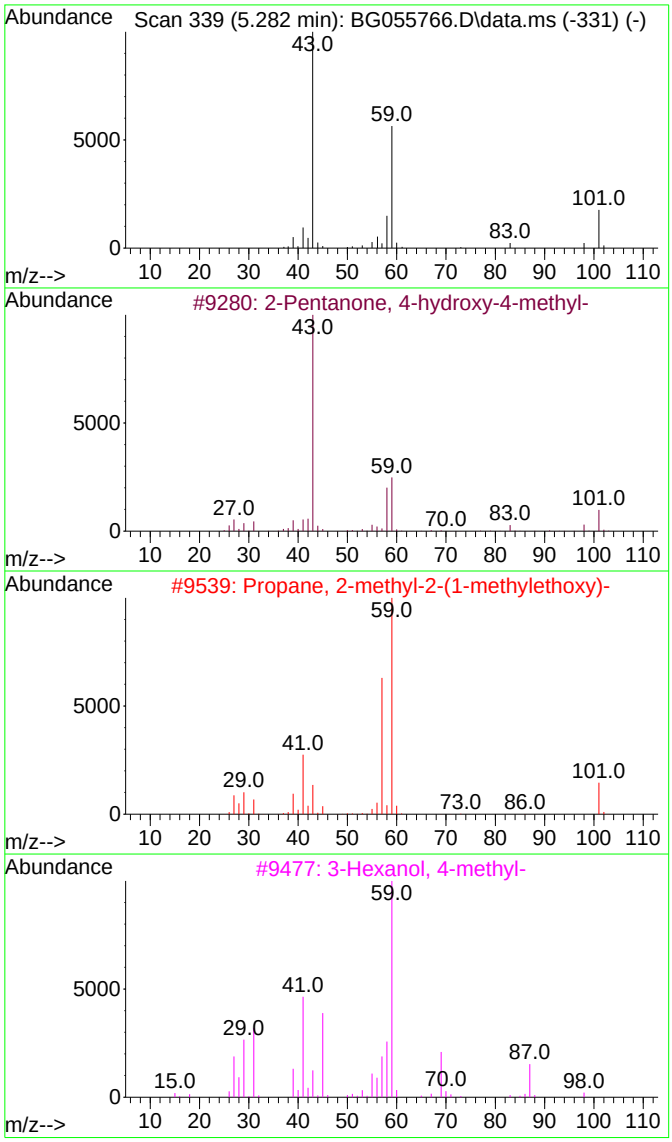
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

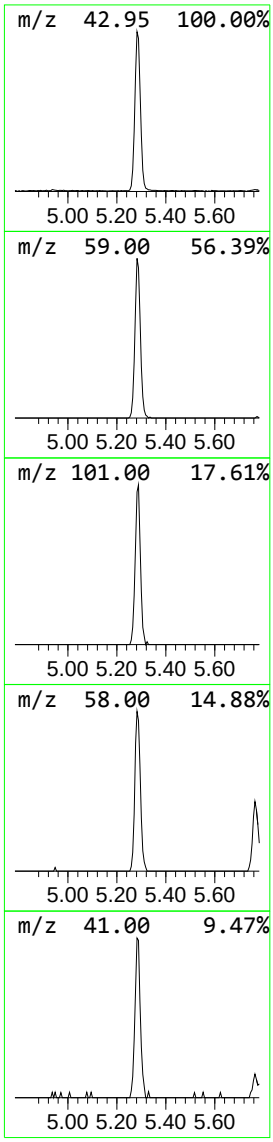
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.282	23.00 ng	192894	1,4-Dichlorobenzene-d4	8.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

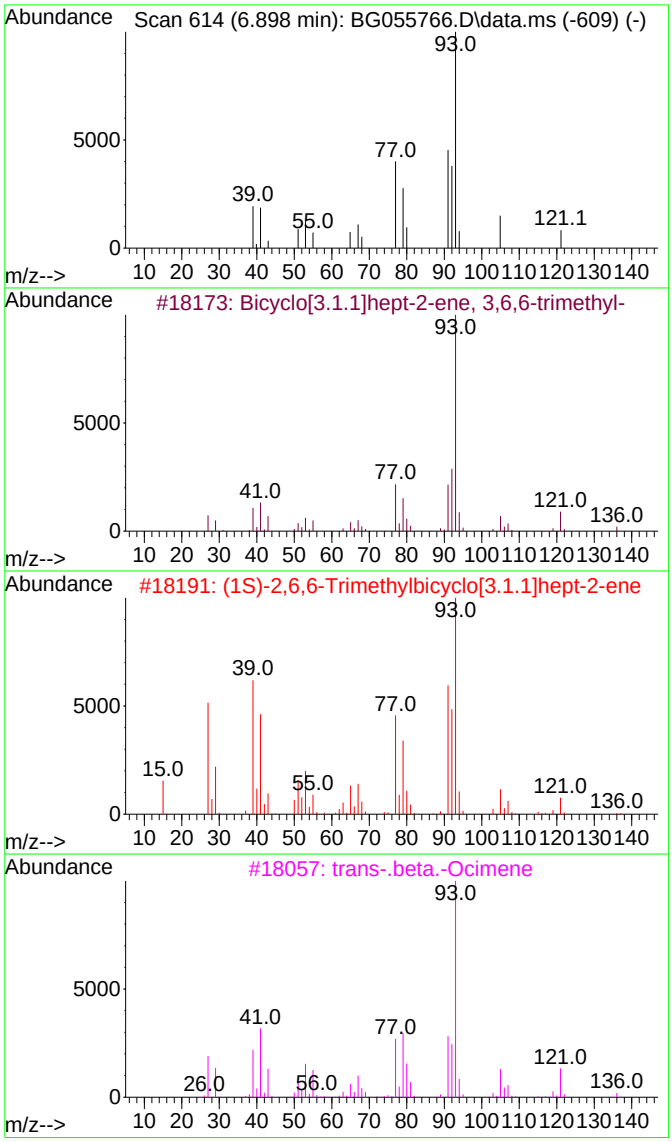
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

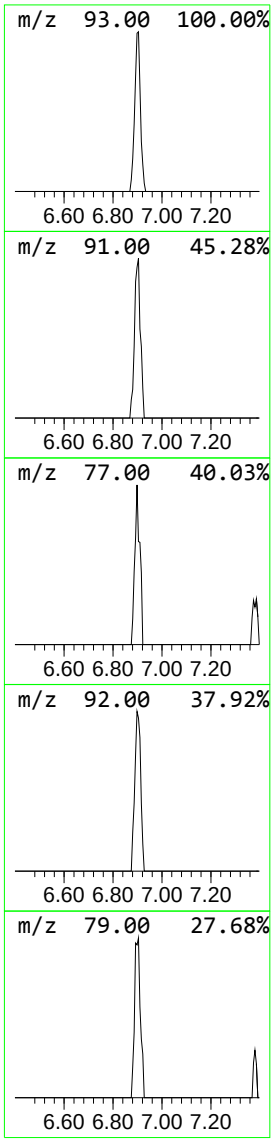
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.898	2.39 ng	20011	1,4-Dichlorobenzene-d4	8.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	78
2	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	64
3	trans-.beta.-Ocimene	136	C10H16	003779-61-1	50
4	1,3-Cyclohexadiene, 5,6-dimethyl-	108	C8H12	005715-27-5	36
5	3,5-Methanocyclopentapyrazole, 3...	164	C10H16N2	087143-58-6	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

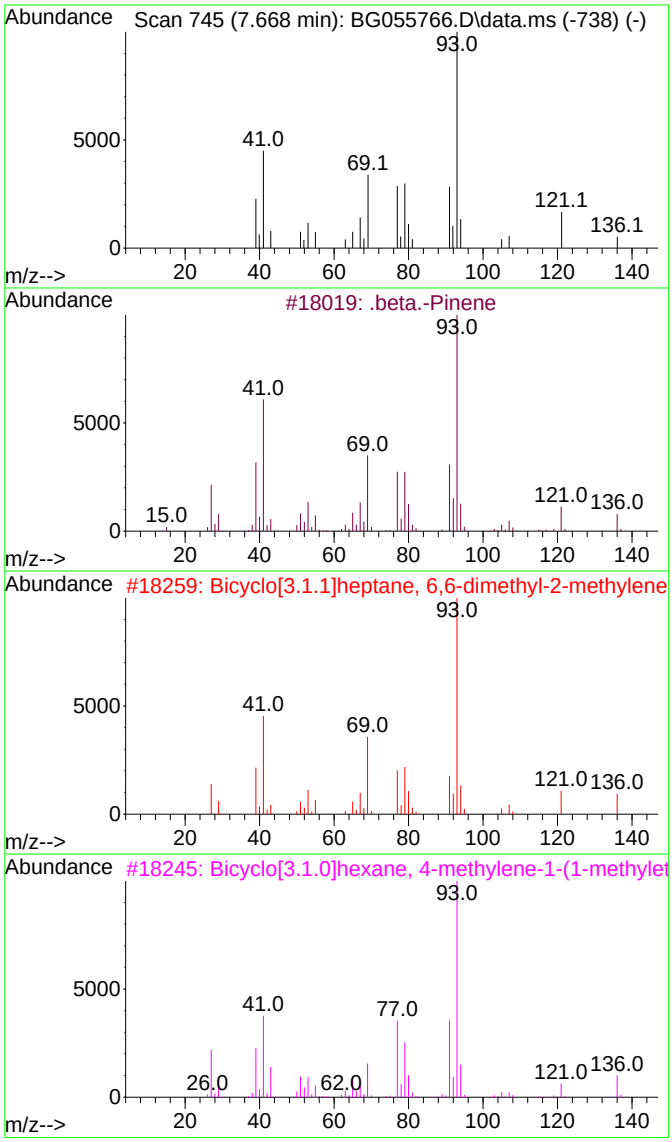
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

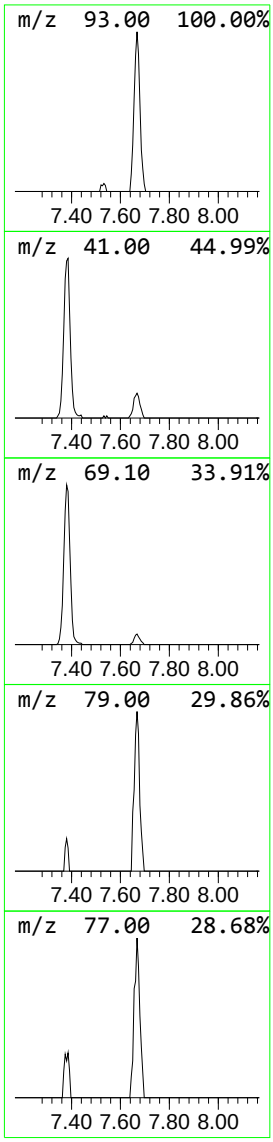
****

Peak Number 3 .beta.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.668	3.50 ng	29363	1,4-Dichlorobenzene-d4	8.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	91
2	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
3	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	87
4	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	83
5	.beta.-Myrcene	136	C10H16	000123-35-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

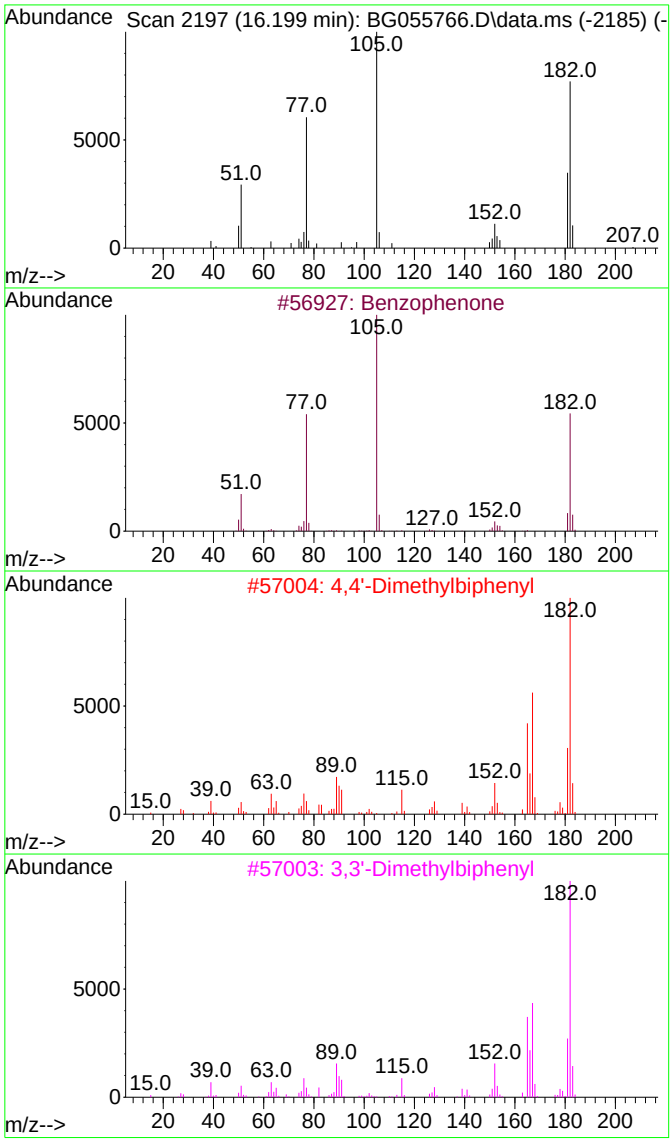
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

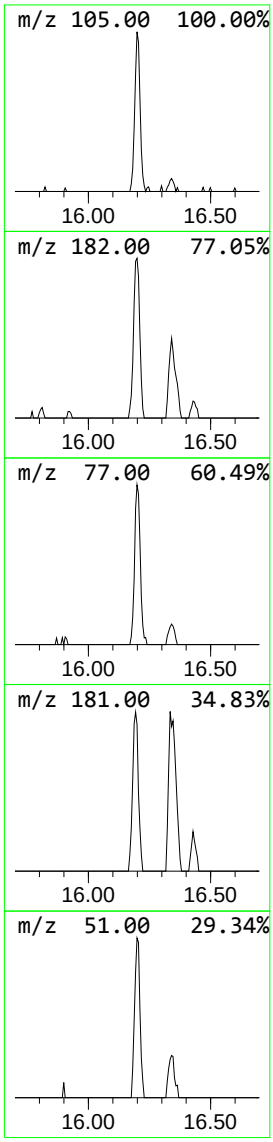
****

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.199	2.39 ng	52542	Acenaphthene-d10	14.859

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	90
2	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	49
3	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	47
4	Phenazine, 5,10-dihydro-	182	C12H10N2	000613-32-1	47
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	38





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Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

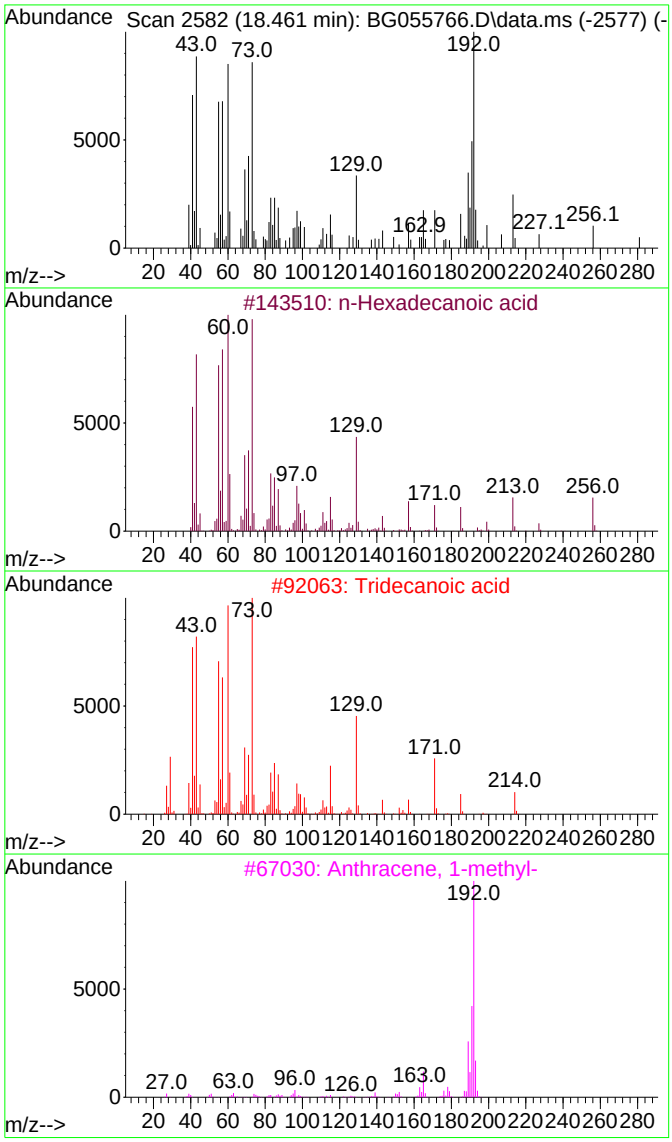
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

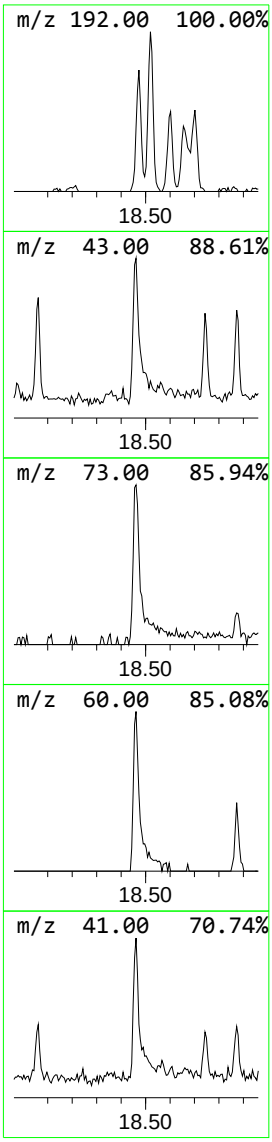
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.461	4.12 ng	114069	Phenanthrene-d10	17.603

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	84
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	47





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Acq On : 23 Nov 2022 22:21
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Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

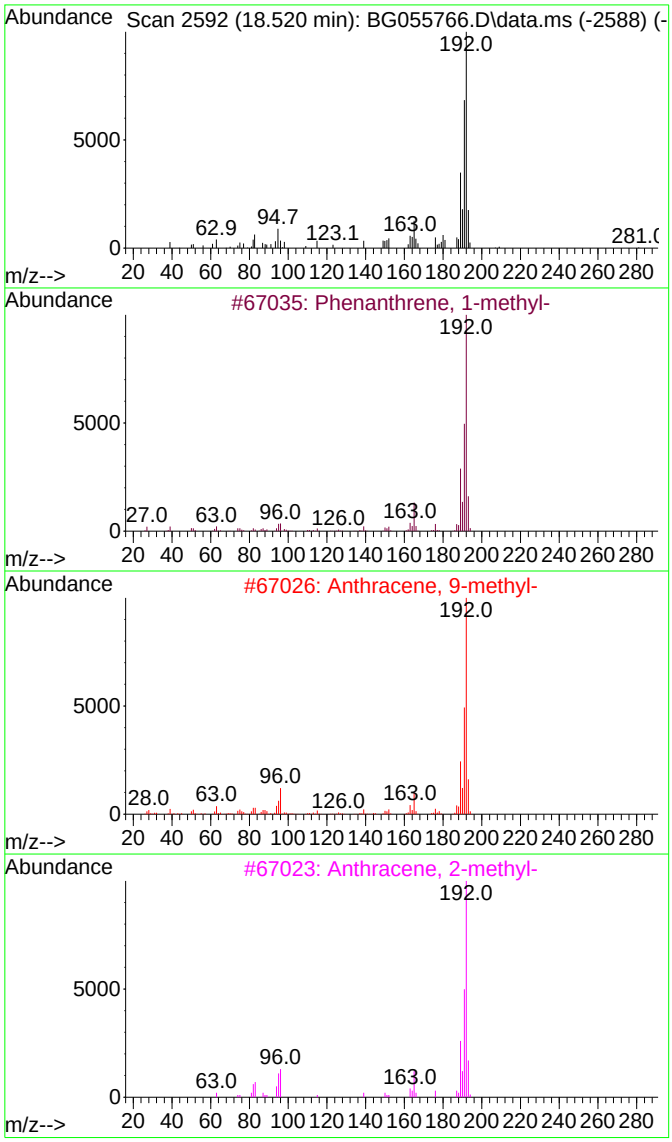
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

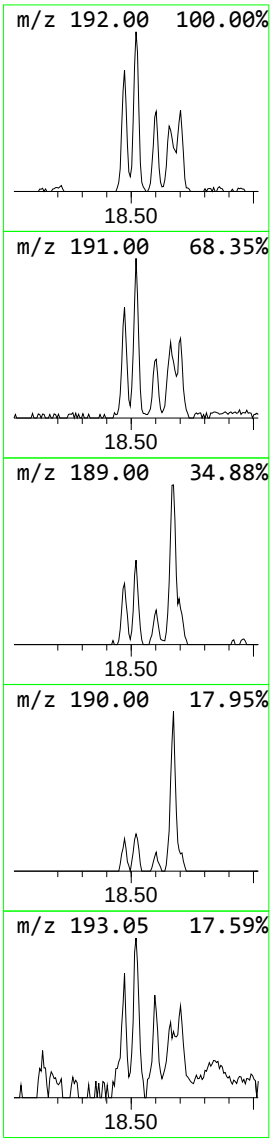
****

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.520	2.36 ng	65191	Phenanthrene-d10	17.603

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87





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Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

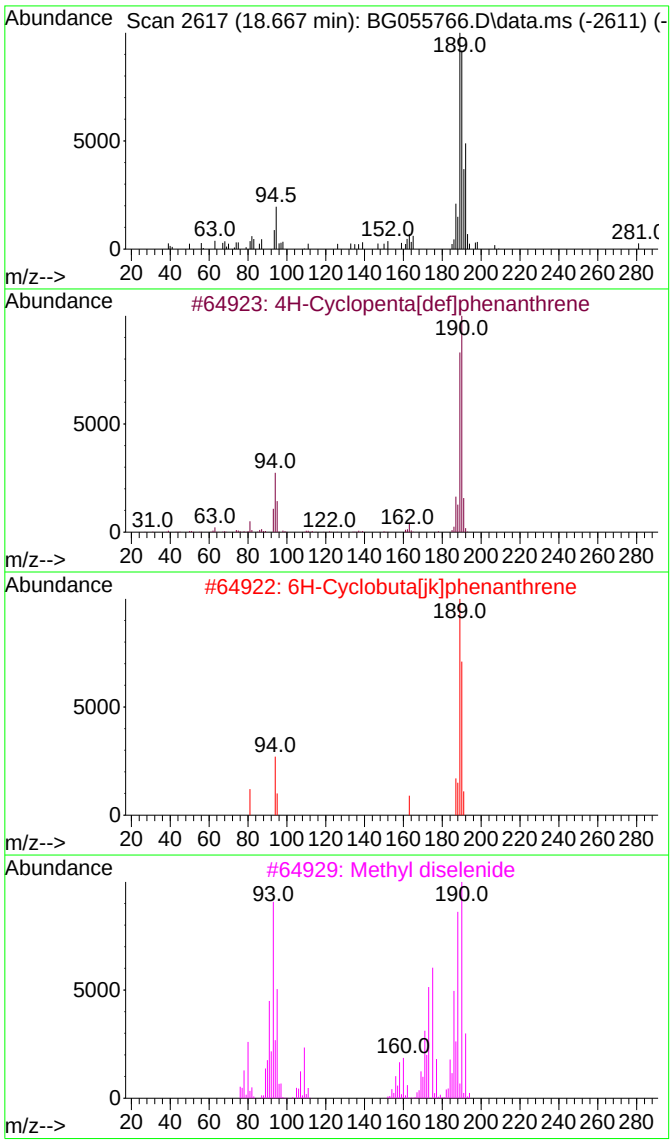
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

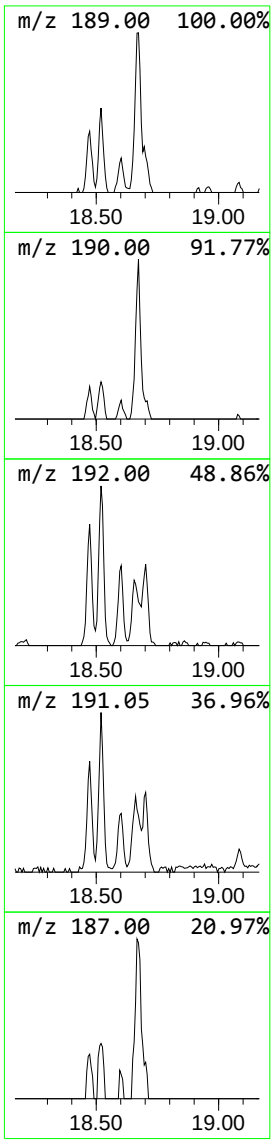
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.667	2.27 ng	62918	Phenanthrene-d10	17.603

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

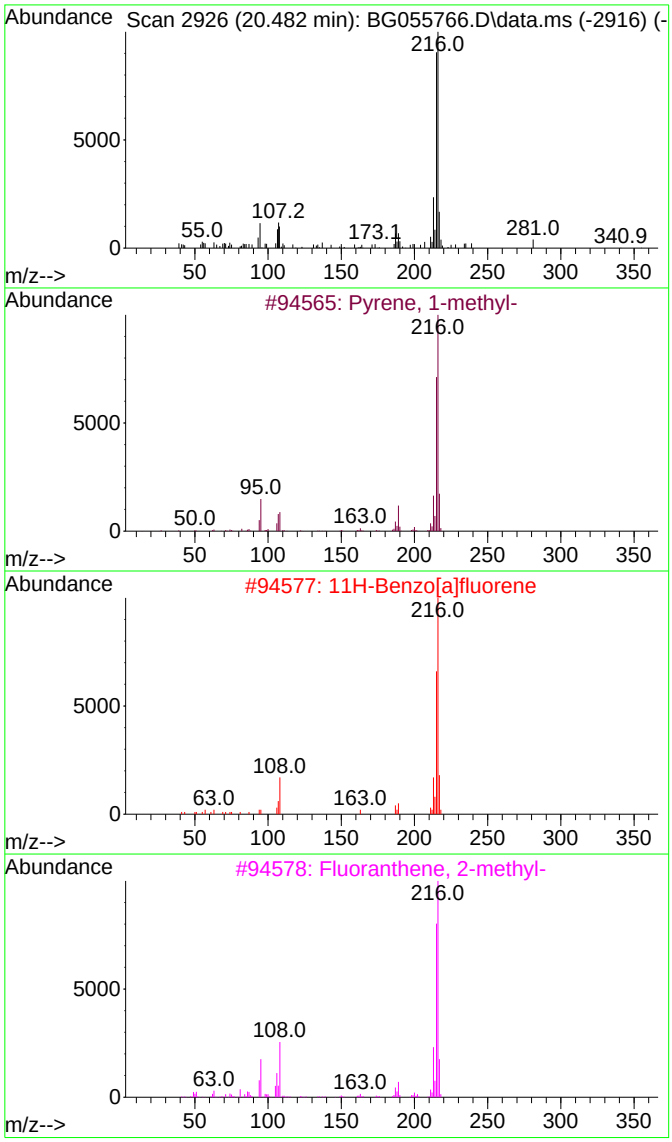
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

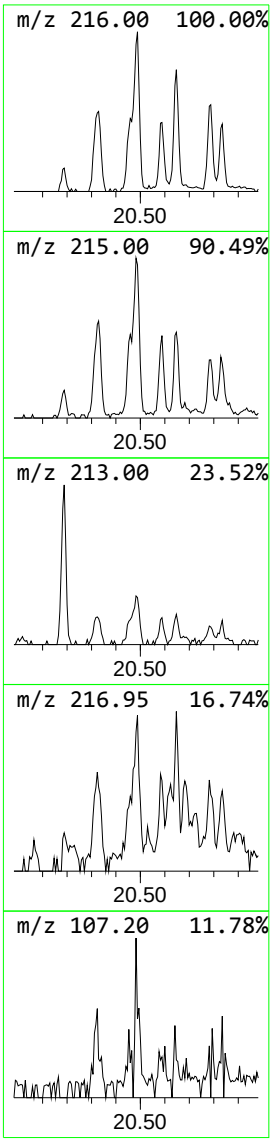
****

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.482	2.16 ng	92256	Chrysene-d12	21.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

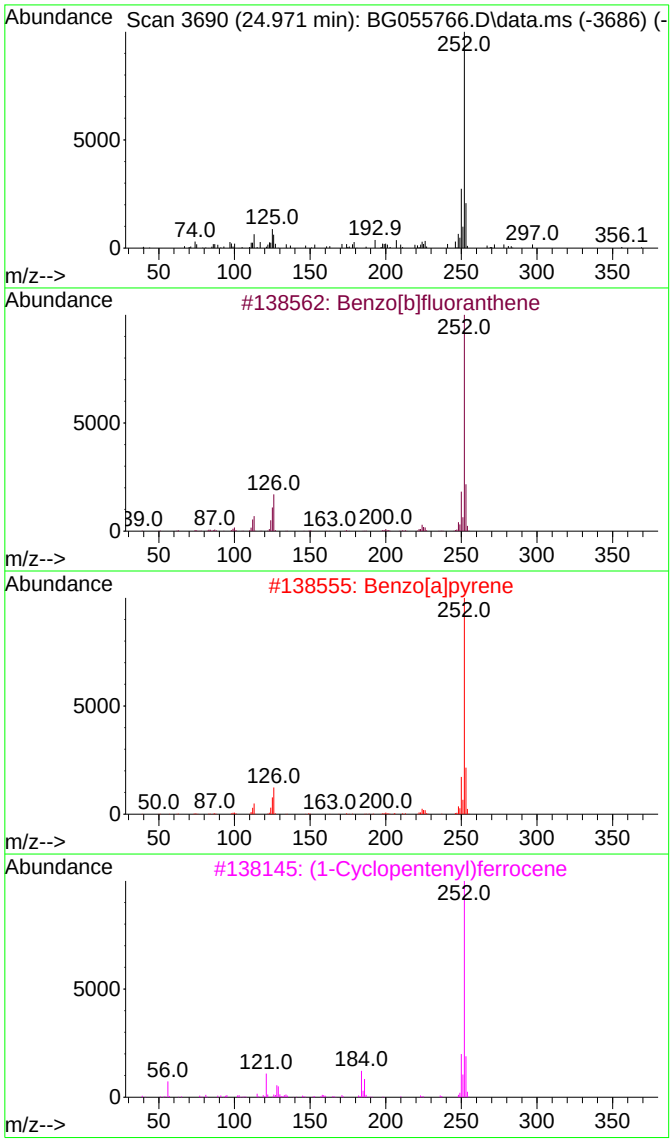
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

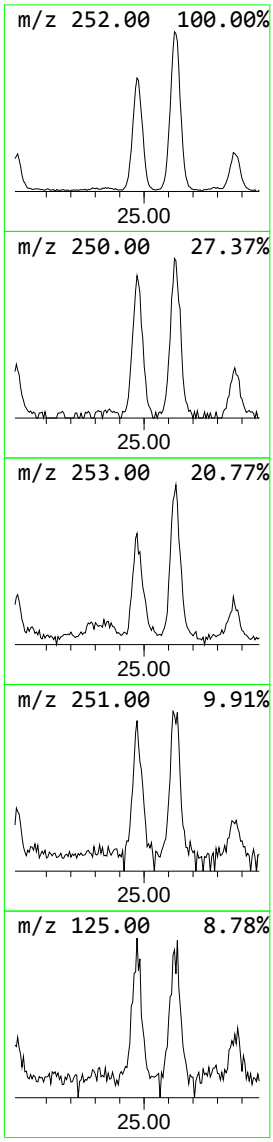
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (1-Cyclopentenyl)ferrocene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.971	2.89 ng	98878	Perylene-d12	25.294

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
2	Benzo[a]pyrene	252	C20H12	000050-32-8	81
3	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	78
4	Benzo[e]pyrene	252	C20H12	000192-97-2	76
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112322\
Data File : BG055766.D
Acq On : 23 Nov 2022 22:21
Operator : CG/JU
Sample : N5754-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.282	23.0	ng	192894	1	8.238	167763	20.0
Bicyclo[3.1.1]h...	6.898	2.4	ng	20011	1	8.238	167763	20.0
.beta.-Pinene	7.668	3.5	ng	29363	1	8.238	167763	20.0
Benzophenone	16.199	2.4	ng	52542	3	14.859	439391	20.0
n-Hexadecanoic ...	18.461	4.1	ng	114069	4	17.603	553528	20.0
Phenanthrene, 1...	18.520	2.4	ng	65191	4	17.603	553528	20.0
4H-Cyclopenta[d...	18.667	2.3	ng	62918	4	17.603	553528	20.0
Pyrene, 1-methyl-	20.482	2.2	ng	92256	5	21.892	854612	20.0
(1-Cyclopenteny...	24.971	2.9	ng	98878	6	25.294	684832	20.0