LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.332	3	7	14	rVB	38846	51031	2.85%	0.327%
2	4.389	181	187	191	rBV	11352	20025	1.12%	0.128%
3	5.335	340	348	360	rBV	70235	126168	7.04%	0.808%
4	5.799	421	427	440	rBV	252058	456684	25.48%	2.926%
5	6.234	493	501	509	rBV	22566	41786	2.33%	0.268%
6	7.409	693	701	710	rBV	292706	518401	28.93%	3.322%
7	8.279	841	849	861	rVB	276583	496020	27.68%	3.178%
8	9.448	1040	1048	1056	rBV	176359	321261	17.93%	2.058%
9	10.852	1280	1287	1297	rBV	16365	29066	1.62%	0.186%
10	11.105	1321	1330	1338	rBV	399846	736613	41.10%	4.720%
11	12.867	1624	1630	1634	rBV	16823	23230	1.30%	0.149%
12	13.520	1735	1741	1748	rVB	506496	768836	42.90%	4.926%
13	14.319	1873	1877	1884	rBV	11397	17950	1.00%	0.115%
14	14.894	1965	1975	1982	rBV	639316	998464	55.72%	6.397%
15	14.959	1982	1986	1992	rVB	19158	29571	1.65%	0.189%
16	15.282	2035	2041	2049	rVB4	13285	25929	1.45%	0.166%
17	15.670	2100	2107	2111	rBV5	11923	25734	1.44%	0.165%
18	15.934	2146	2152	2157	rBV3	18822	34145	1.91%	0.219%
19	16.099	2176	2180	2185	rVB	15836	22462	1.25%	0.144%
20	16.375	2220	2227	2236	rBV	366574	571090	31.87%	3.659%
21	16.451	2236	2240	2248	rVB5	11680	23332	1.30%	0.149%
22	16.598	2263	2265	2272	rVB6	15263	21586	1.20%	0.138%
23	16.739	2284	2289	2294	rBV8	11466	24816	1.38%	0.159%
24	16.939	2316	2323	2327	rBV9	16003	34569	1.93%	0.221%
25	16.986	2328	2331	2337	rVB5	9120	18036	1.01%	0.116%
26	17.086	2345	2348	2354	rVB8	13098	19390	1.08%	0.124%
27	17.227	2370	2372	2376	rVB2	19636	21535	1.20%	0.138%
28	17.286	2378	2382	2387	rVB4	22267	33121	1.85%	0.212%
29	17.368	2391	2396	2398	rBV6	14469	20173	1.13%	0.129%
30	17.450	2407	2410	2415	rBV	19520	29198	1.63%	0.187%
31	17.638	2435	2442	2446	rBV	690501	1130197	63.07%	7.242%
32	17.679	2446	2449	2455	rVB	336414	472725	26.38%	3.029%
33	17.768	2460	2464	2468	rVV	65027	93187	5.20%	0.597%
34	18.032	2505	2509	2511	rBV2	23079	33344	1.86%	0.214%
35	18.149	2526	2529	2533	rBV3	18566	30203	1.69%	0.194%
36	18.214	2536	2540	2548	rVB3	34511	66756	3.73%	0.428%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.355	2561	2564	2569	rBV2	16711	28821	1.61%	0.185%
38	18.508	2583	2590	2594	rBV2	140413	276805	15.45%	1.774%
39	18.567	2594	2600	2606	rVB2	168992	388180	21.66%	2.487%
40	18.649	2608	2614	2617	rBV3	55894	112759	6.29%	0.722%
41	18.696	2617	2622	2626	rBV2	134810	241109	13.45%	1.545%
42	18.737	2626	2629	2634	rVB2	73890	114419	6.38%	0.733%
43	18.996	2669	2673	2676	rBV	68106	96524	5.39%	0.618%
44	19.037	2677	2680	2685	rVB3	53749	83197	4.64%	0.533%
45	19.125	2691	2695	2697	rBV	28052	42055	2.35%	0.269%
46	19.236	2712	2714	2718	rVB2	50436	55009	3.07%	0.352%
47	19.289	2720	2723	2726	rBV	38534	42860	2.39%	0.275%
48	19.330	2726	2730	2737	rVB4	59528	96522	5.39%	0.618%
49	19.407	2738	2743	2748	rBV	182311	309807	17.29%	1.985%
50	19.466	2749	2753	2757	rBV3	76835	122092	6.81%	0.782%
51	19.548	2763	2767	2773	rBV3	91718	184713	10.31%	1.184%
52	19.671	2783	2788	2794	rVB	611275	868371	48.46%	5.564%
53	19.900	2824	2827	2832	rBV3	130408	183140	10.22%	1.173%
54	20.036	2840	2850	2857	rBV	758207	1294480	72.23%	8.294%
55	20.218	2877	2881	2886	rBV	701912	875608	48.86%	5.610%
56	20.676	2957	2959	2963	rVB	134701	161904	9.03%	1.037%
57	20.817	2980	2983	2987	rBV	142021	177976	9.93%	1.140%
58	20.864	2988	2991	2995	rVB	99579	124649	6.96%	0.799%
59	21.933	3165	3173	3179	rBV2	697012	1792043	100.00%	11.482%
60	21.986	3179	3182	3190	rVB	329510	547422	30.55%	3.508%

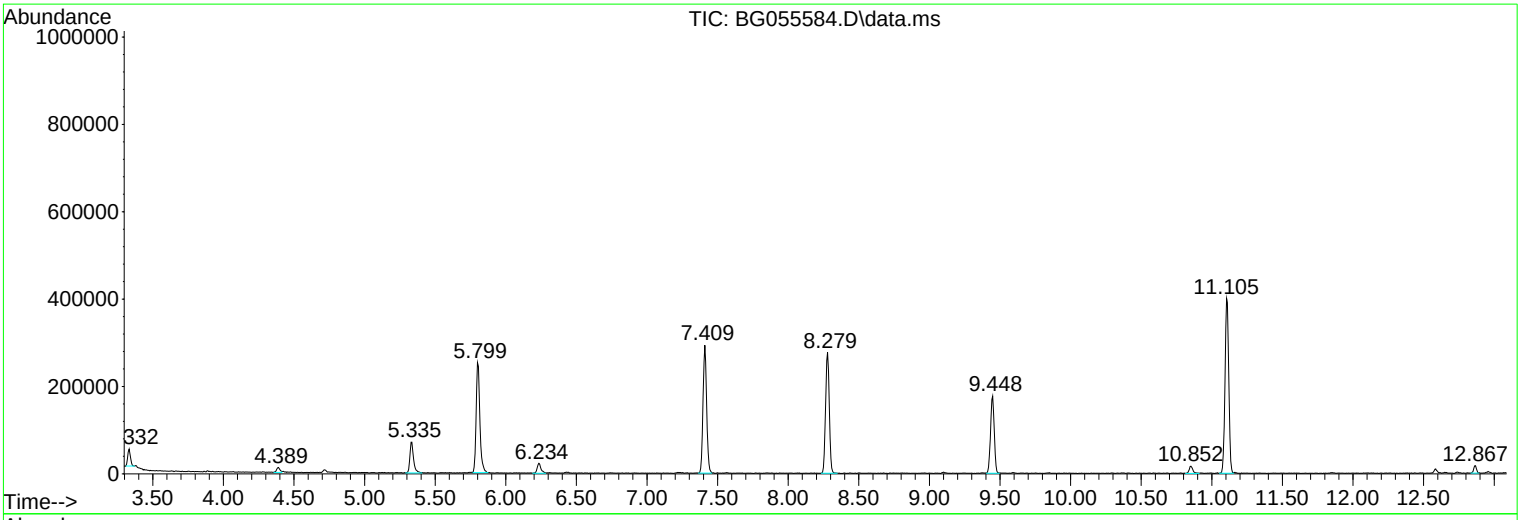
Sum of corrected areas: 15607099

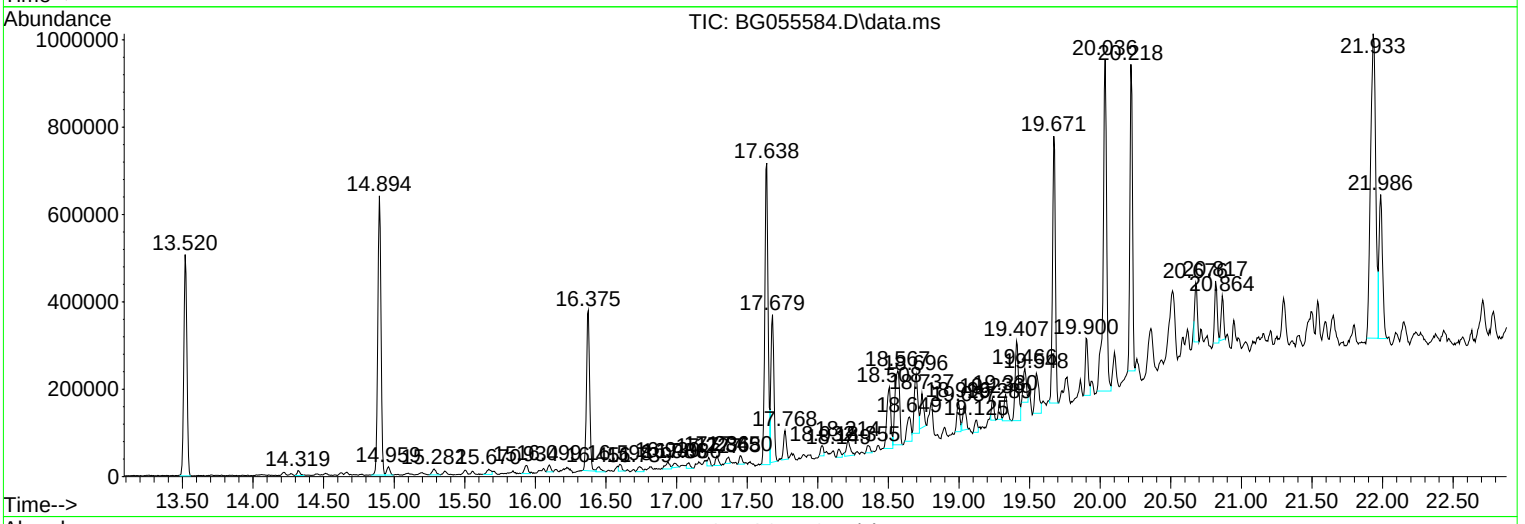
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

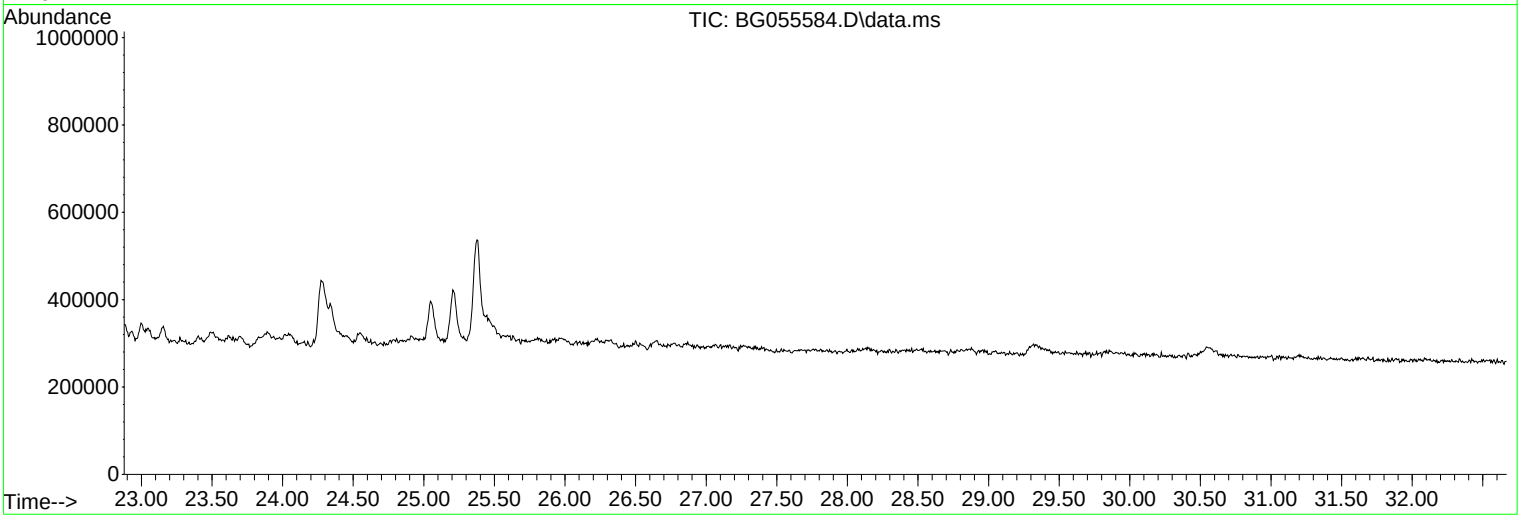
Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
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Misc :
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

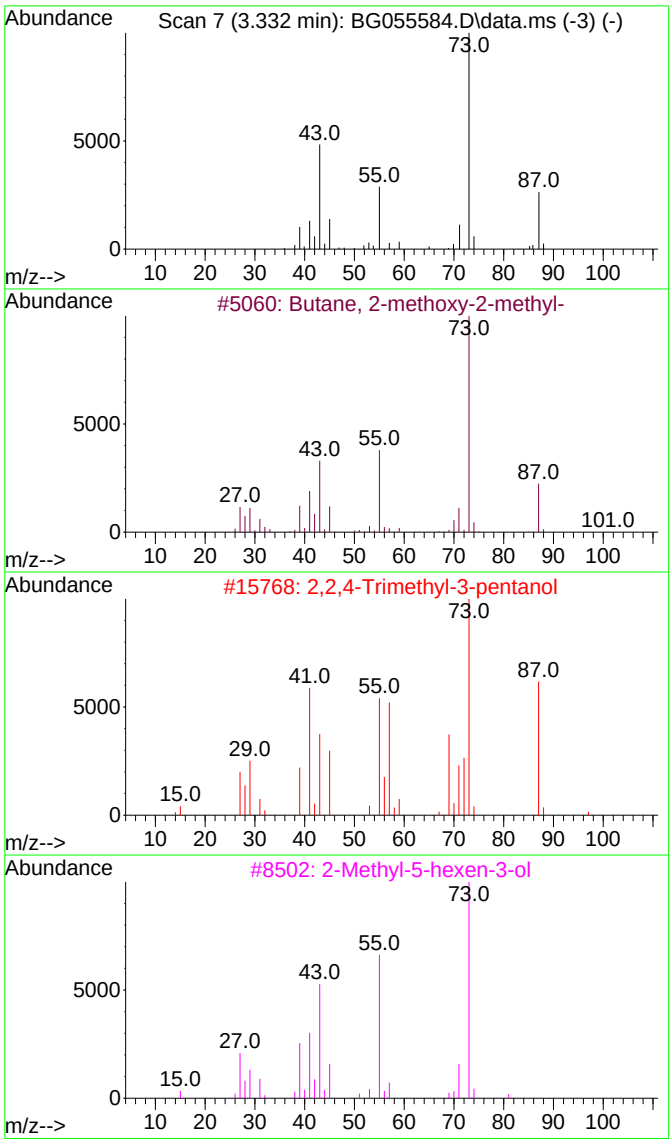
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

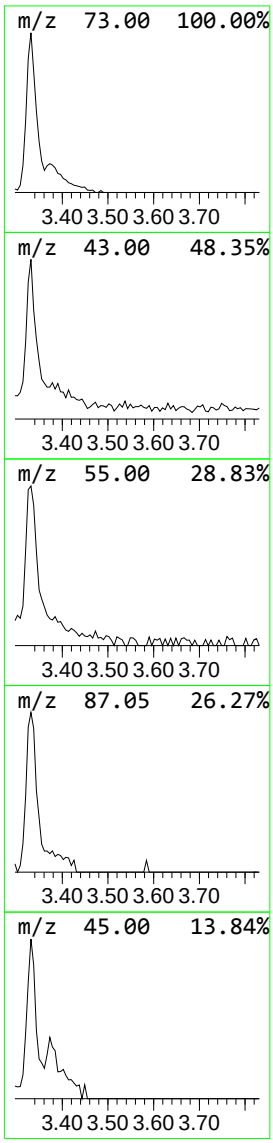
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.332	2.06 ng	51031	1,4-Dichlorobenzene-d4	8.279

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	45
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

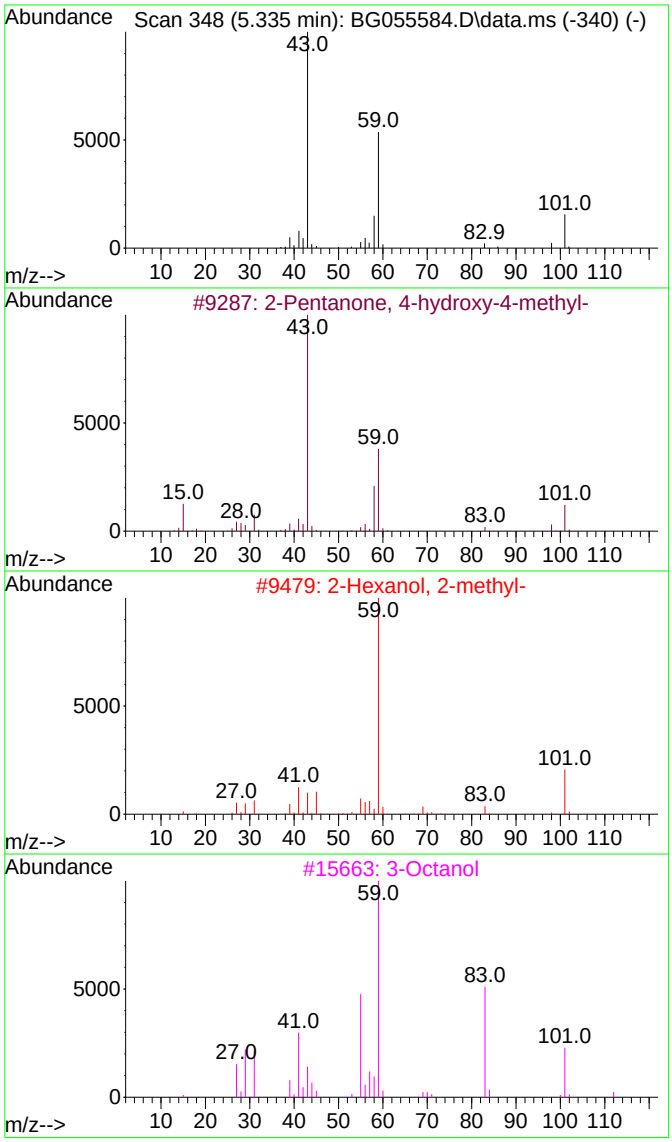
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

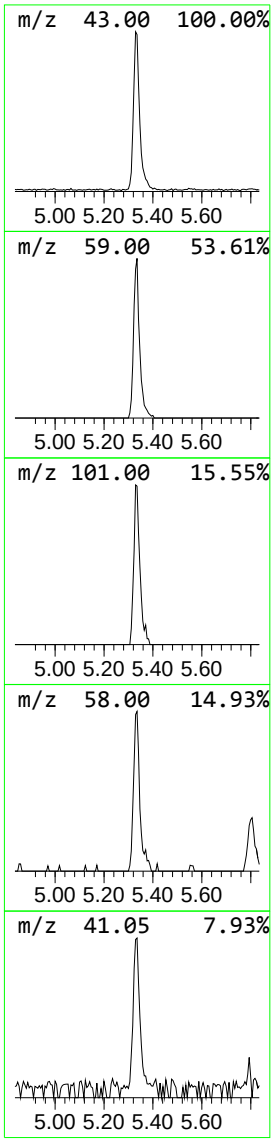
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.335	5.09 ng	126168	1,4-Dichlorobenzene-d4	8.279

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	3-Octanol	130	C8H18O	000589-98-0	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

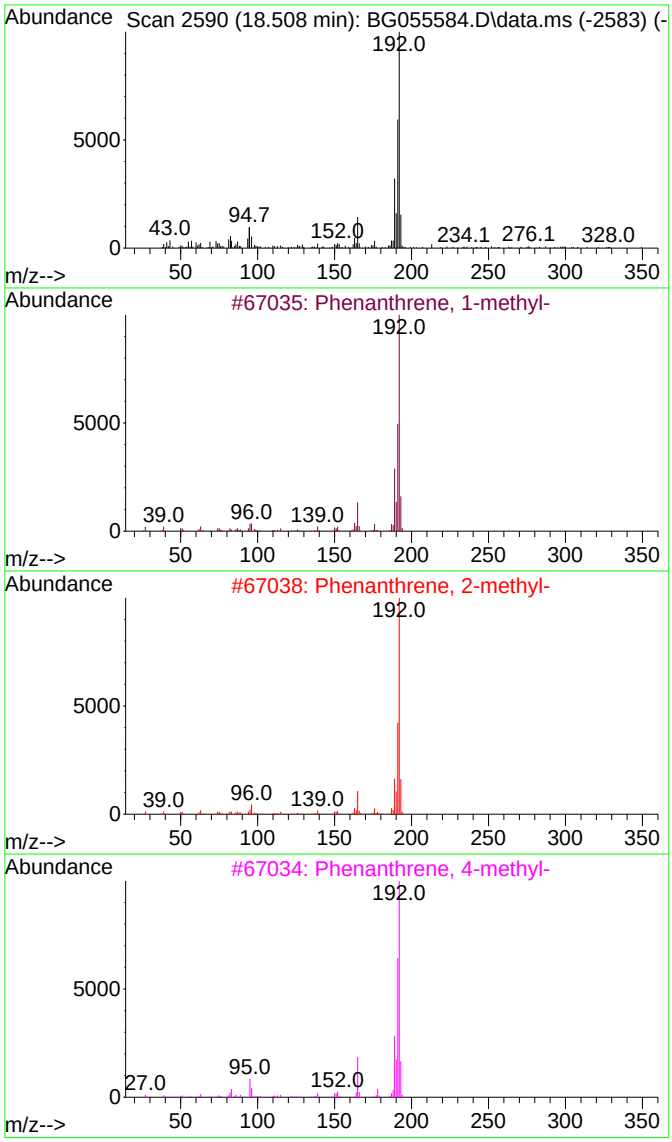
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

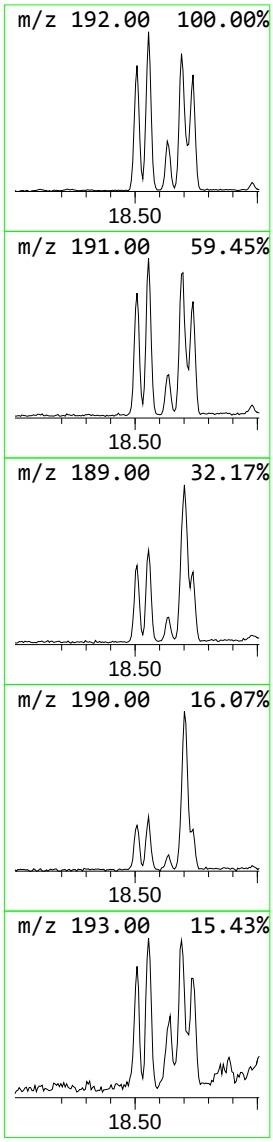
****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.508	4.90 ng	276805	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

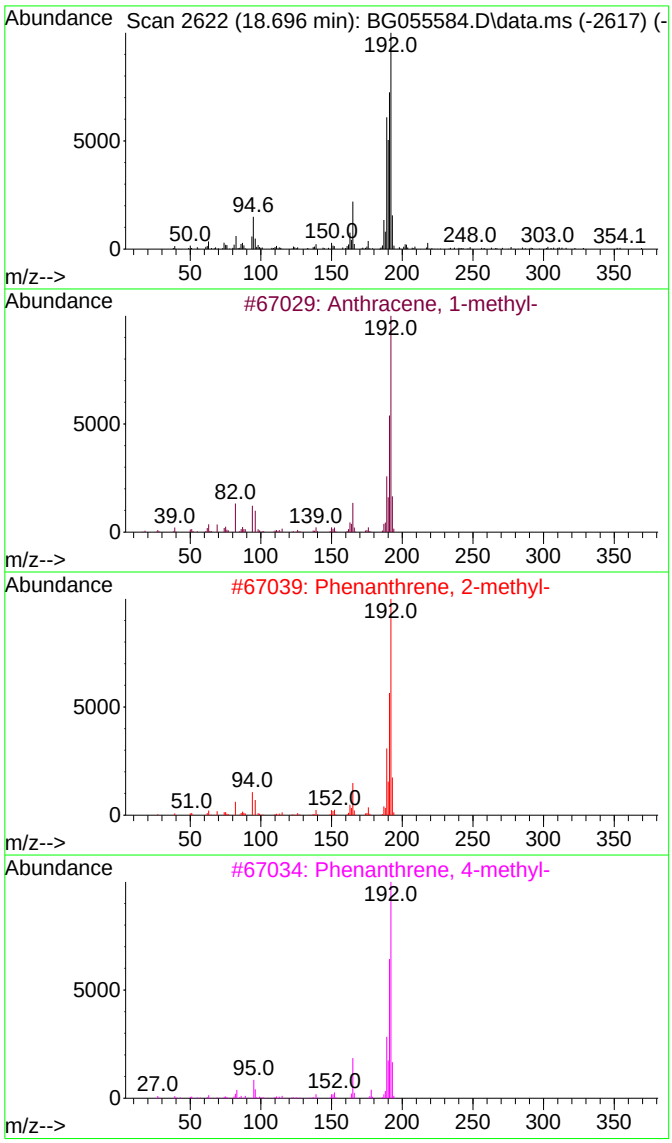
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

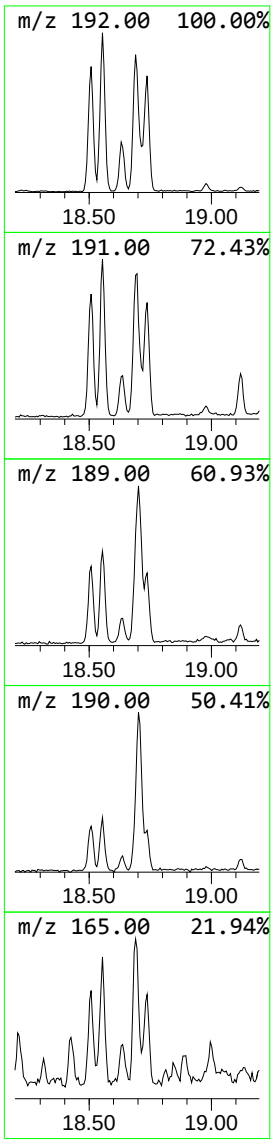
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.696	4.27 ng	241109	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

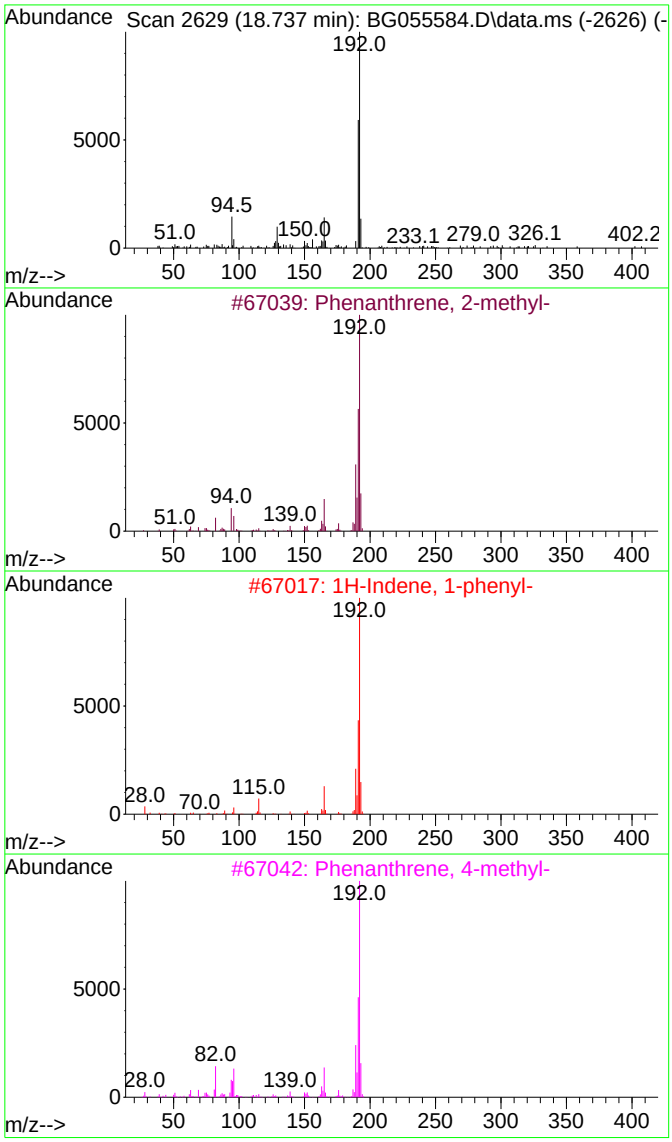
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

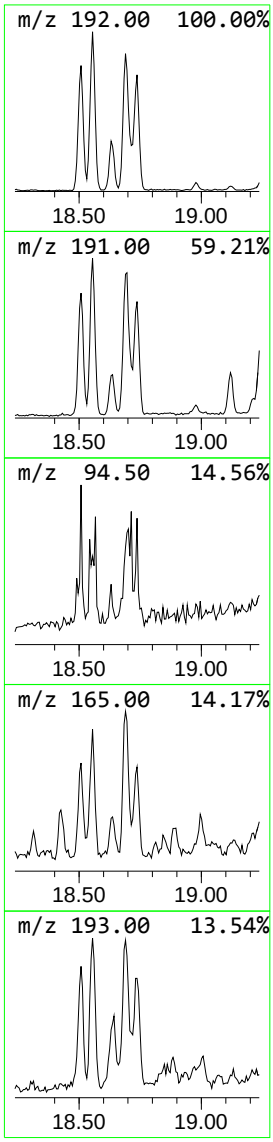
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.737	2.02 ng	114419	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	83
2	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	81
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	80
4	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	74
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

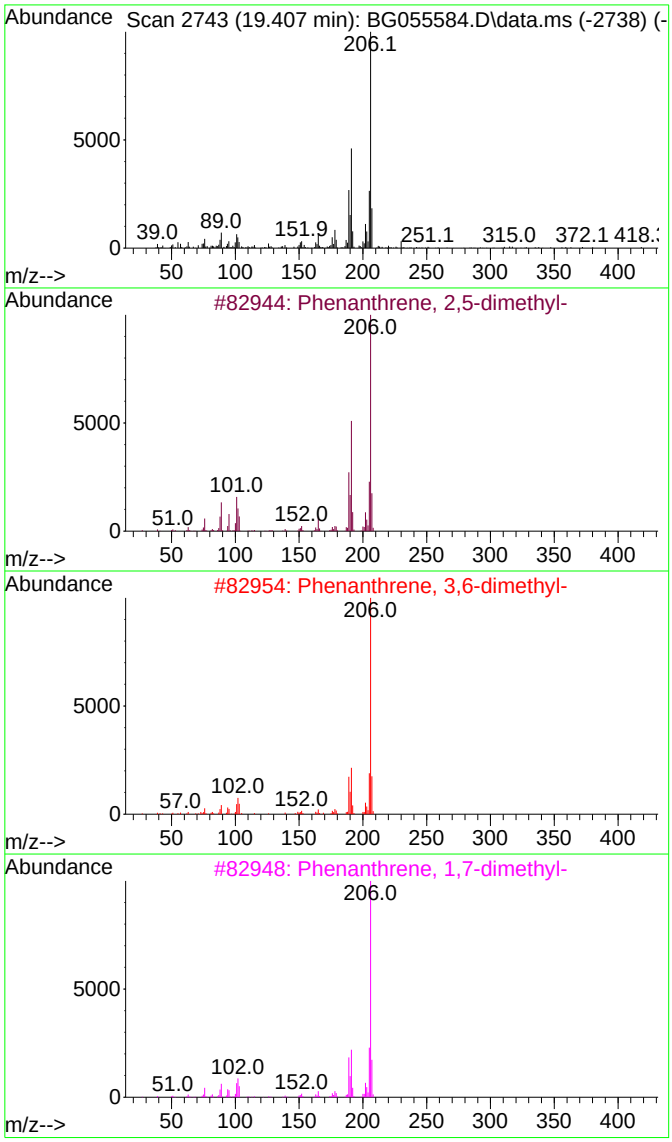
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

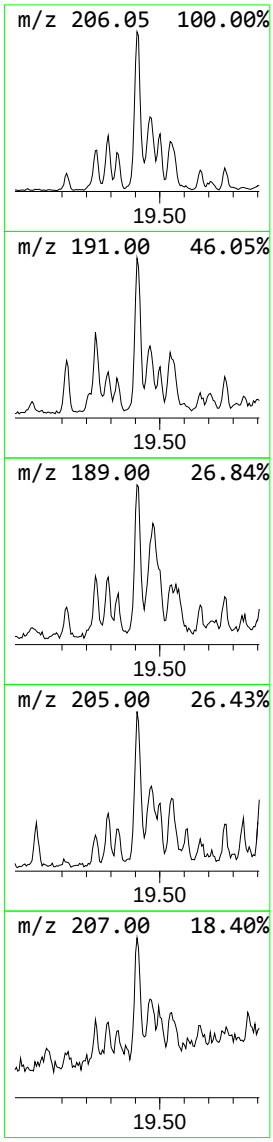
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.407	5.48 ng	309807	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
3	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90
4	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90
5	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

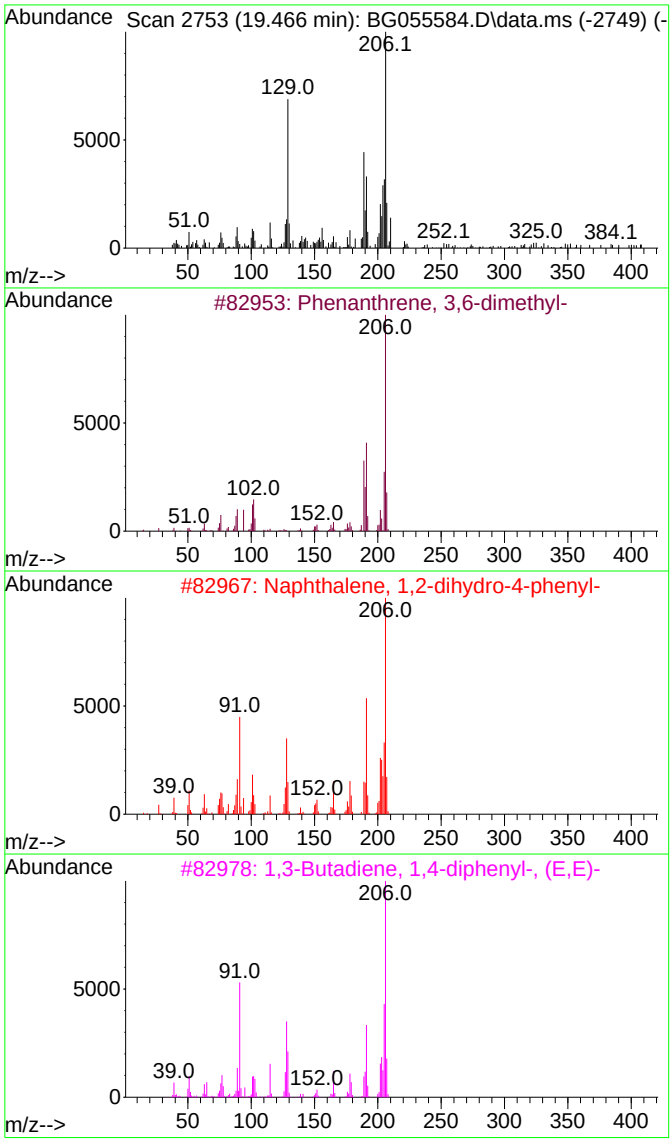
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

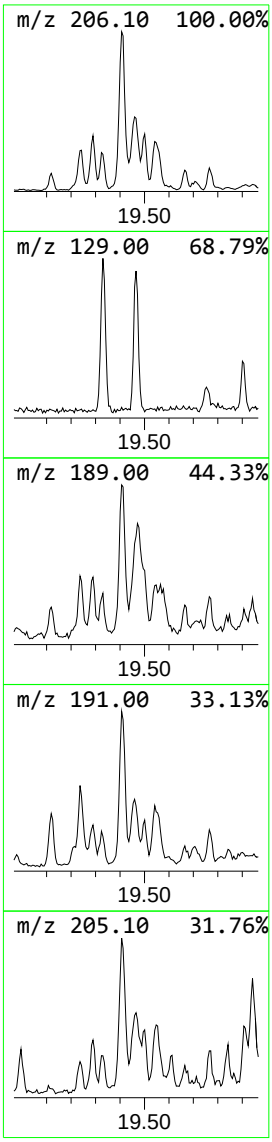
****

Peak Number 7 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.466	2.16 ng	122092	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	70
2	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	64
3	1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	64
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	55
5	1,2-Dihydro-3-phenylnaphthalene	206	C16H14	020669-52-7	55





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Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

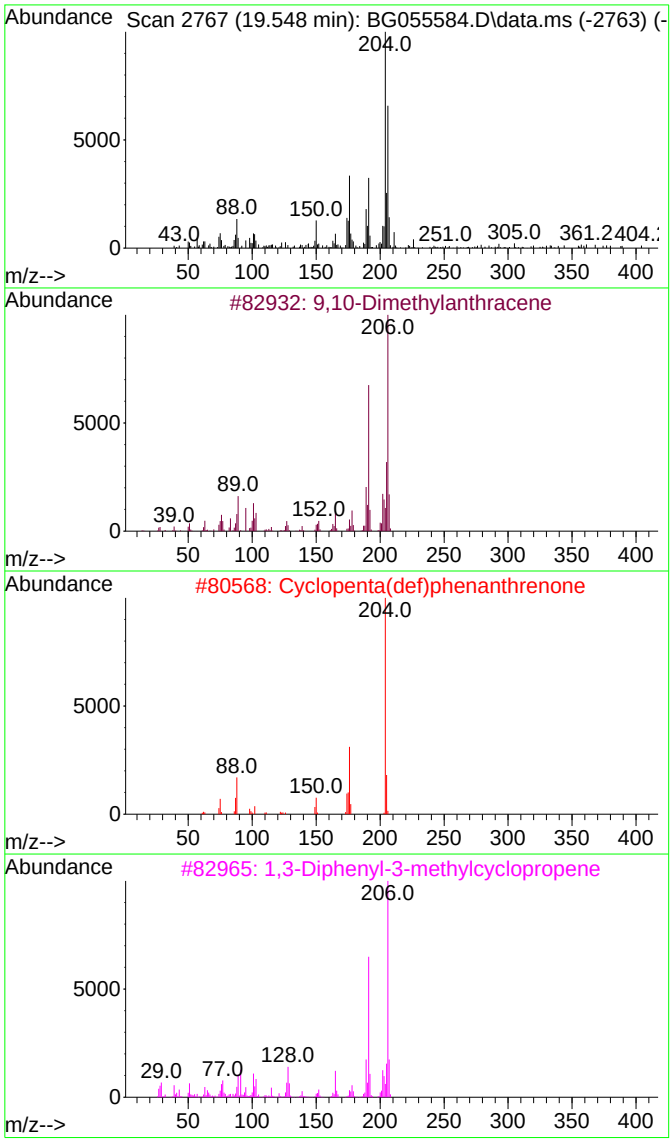
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

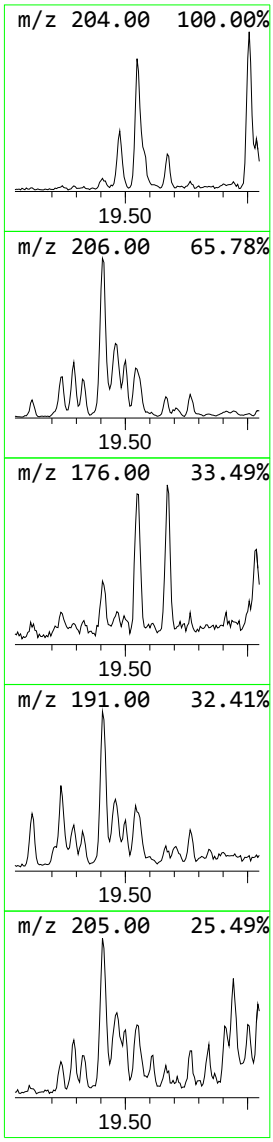
****

Peak Number 8 9,10-Dimethylanthracene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.548	3.27 ng	184713	Phenanthrene-d10	17.638

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	87
2	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	55
3	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	52
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	46
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

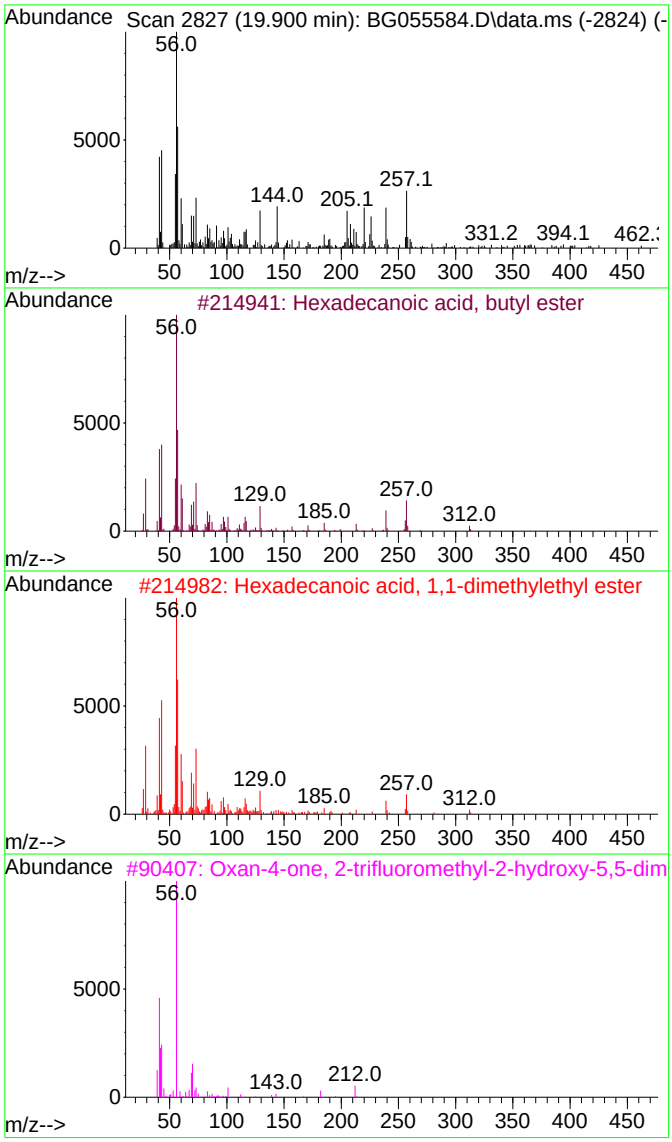
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

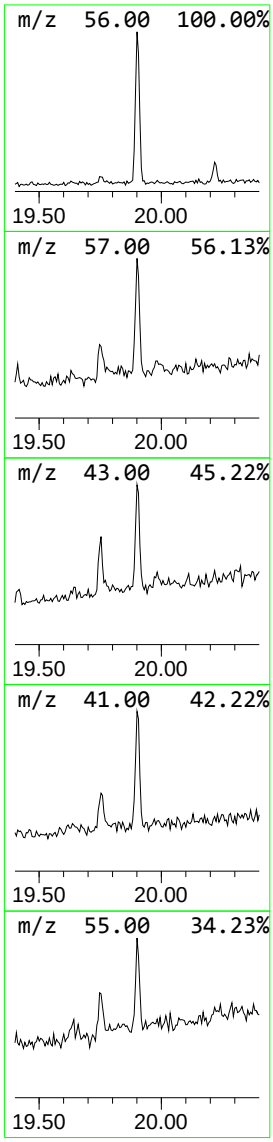
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.900	2.04 ng	183140	Chrysene-d12	21.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	62
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Oxan-4-one, 2-trifluoromethyl-2-...	212	C8H11F3O3	212615-80-0	35
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	30
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055584.D
Acq On : 12 Nov 2022 3:17
Operator : CG/JU
Sample : N5531-15 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.332	2.1	ng	51031	1	8.279	496020	20.0
2-Pentanone, 4-...	5.335	5.1	ng	126168	1	8.279	496020	20.0
Phenanthrene, 1...	18.508	4.9	ng	276805	4	17.638	1130200	20.0
Anthracene, 1-m...	18.696	4.3	ng	241109	4	17.638	1130200	20.0
Phenanthrene, 2...	18.737	2.0	ng	114419	4	17.638	1130200	20.0
Phenanthrene, 2...	19.407	5.5	ng	309807	4	17.638	1130200	20.0
Phenanthrene, 3...	19.466	2.2	ng	122092	4	17.638	1130200	20.0
9,10-Dimethylan...	19.548	3.3	ng	184713	4	17.638	1130200	20.0
Hexadecanoic ac...	19.900	2.0	ng	183140	5	21.939	1792040	20.0