LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054430.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.105	15	20	30	rVB	75632	119711	4.29%	0.930%
2	5.561	431	438	448	rBV	235095	394463	14.13%	3.065%
3	7.171	705	712	728	rVB	246897	433378	15.53%	3.367%
4	7.988	844	851	858	rBV	56366	98242	3.52%	0.763%
5	9.151	1041	1049	1061	rBB	149827	273802	9.81%	2.128%
6	10.796	1321	1329	1337	rBV	77697	142896	5.12%	1.110%
7	13.246	1739	1746	1754	rVB	474063	773829	27.73%	6.013%
8	14.621	1970	1980	1987	rBV	141984	225536	8.08%	1.752%
9	16.114	2226	2234	2246	rBV2	463566	729763	26.15%	5.670%
10	17.371	2441	2448	2451	rBV	183858	294201	10.54%	2.286%
11	17.412	2451	2455	2461	rVV	107209	166433	5.96%	1.293%
12	17.500	2465	2470	2476	rVV	36961	54649	1.96%	0.425%
13	18.252	2593	2598	2601	rBV2	35912	59594	2.14%	0.463%
14	18.293	2601	2605	2611	rVB2	31770	51639	1.85%	0.401%
15	18.440	2625	2630	2634	rBV2	33027	62138	2.23%	0.483%
16	19.157	2748	2752	2755	rBV3	17354	28000	1.00%	0.218%
17	19.421	2792	2797	2803	rVB	312603	444686	15.93%	3.455%
18	19.486	2804	2808	2812	rBV	54041	72112	2.58%	0.560%
19	19.656	2833	2837	2847	rVB3	34141	61519	2.20%	0.478%
20	19.786	2848	2859	2866	rBV2	290429	552401	19.79%	4.292%
21	19.880	2872	2875	2880	rVB	43110	59876	2.15%	0.465%
22	19.980	2885	2892	2899	rBV2	1263568	2117908	75.89%	16.457%
23	20.185	2924	2927	2931	rVB	22622	29245	1.05%	0.227%
24	20.273	2933	2942	2947	rVB	49676	103969	3.73%	0.808%
25	20.397	2955	2963	2968	rBV	2061208	2790829	100.00%	21.686%
26	20.438	2968	2970	2974	rVB2	42760	50466	1.81%	0.392%
27	20.620	2998	3001	3005	rVB	18611	28998	1.04%	0.225%
28	20.826	3032	3036	3040	rBV	88628	119468	4.28%	0.928%
29	20.961	3055	3059	3067	rVB	83481	124812	4.47%	0.970%
30	21.037	3069	3072	3078	rVB	22578	32808	1.18%	0.255%
31	21.266	3107	3111	3115	rBV2	46776	67864	2.43%	0.527%
32	21.631	3165	3173	3178	rBV3	269695	656081	23.51%	5.098%
33	21.678	3178	3181	3193	rVB	141089	239838	8.59%	1.864%
34	21.830	3204	3207	3214	rVB2	28291	47625	1.71%	0.370%
35	23.822	3538	3546	3553	rBV	106635	342360	12.27%	2.660%
36	24.545	3662	3669	3679	rVB2	65145	196023	7.02%	1.523%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.686	3685	3693	3705	rVB	102127	302474	10.84%	2.350%
38	24.839	3711	3719	3727	rBV2	117214	324475	11.63%	2.521%
39	28.511	4338	4344	4360	rVB3	50168	195370	7.00%	1.518%

Sum of corrected areas: 12869481

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
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Acq On : 28 Jul 2022 13:41
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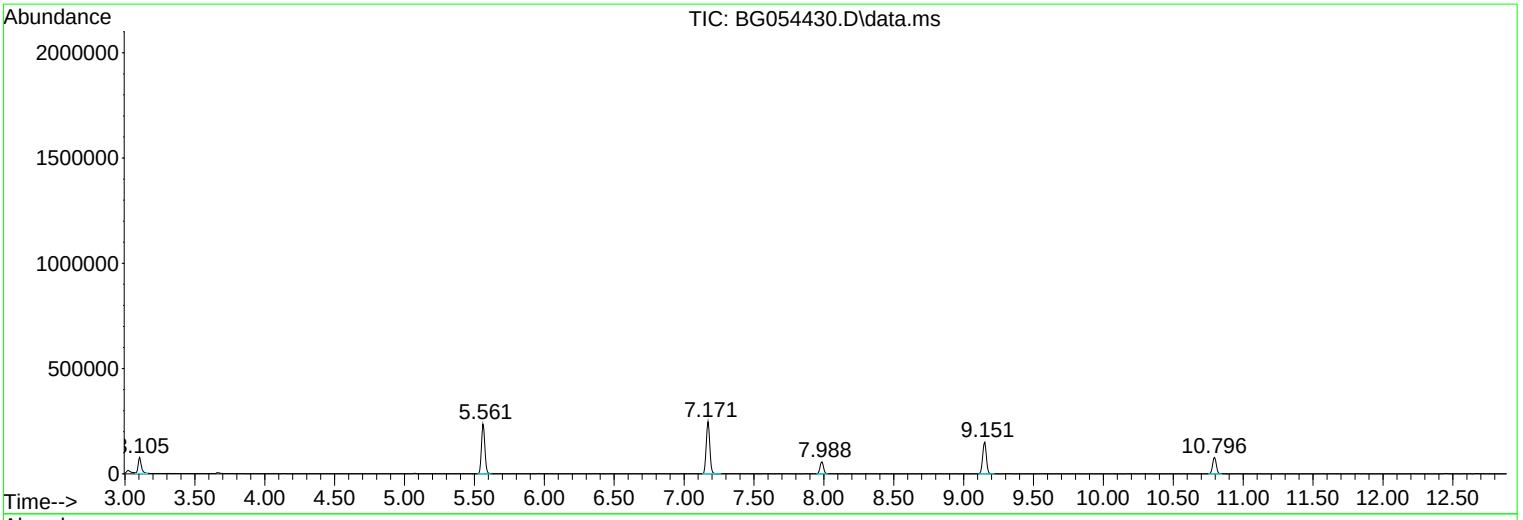
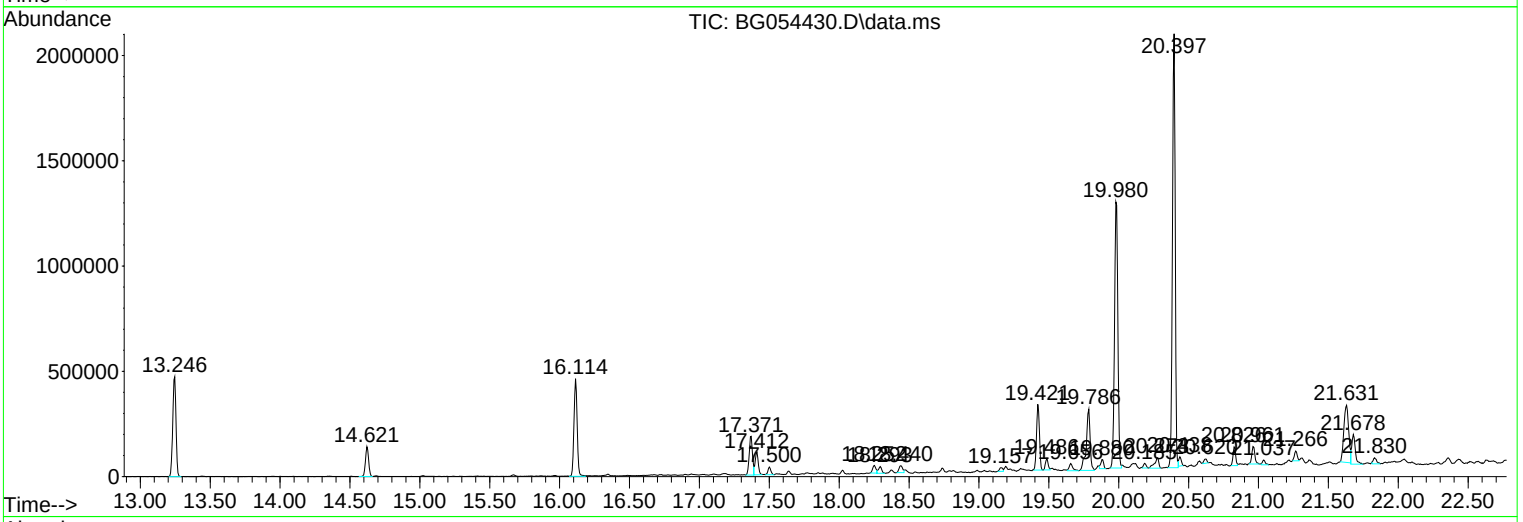
Misc :
ALS Vial : 6 Sample Multiplier: 1

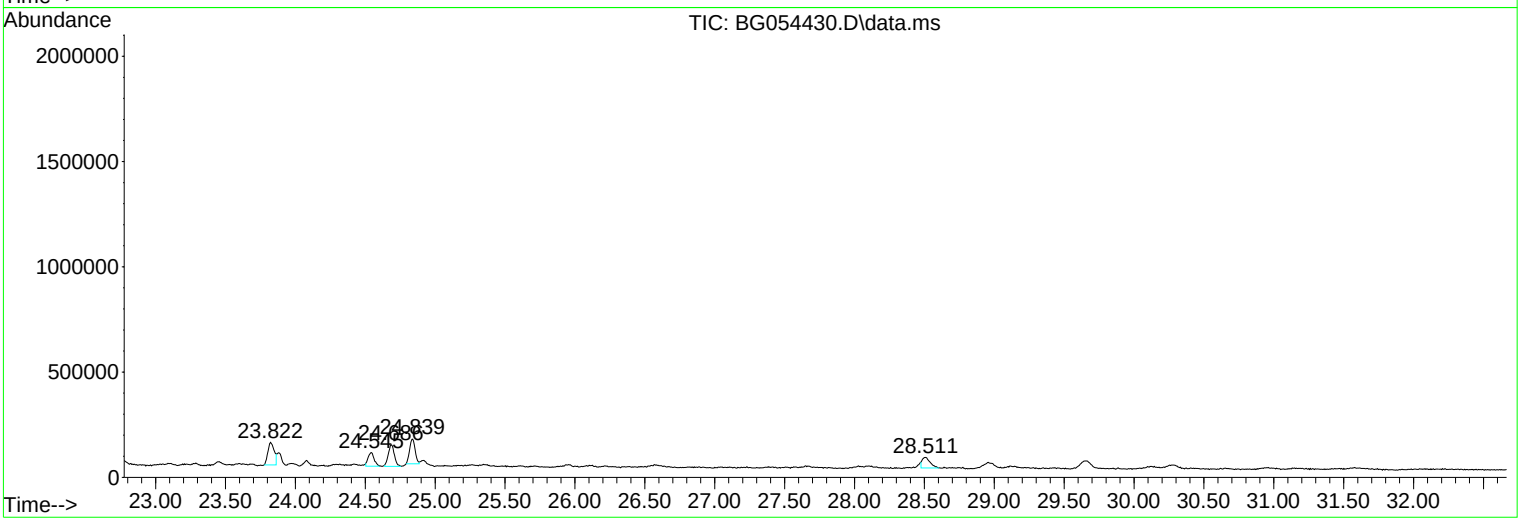
Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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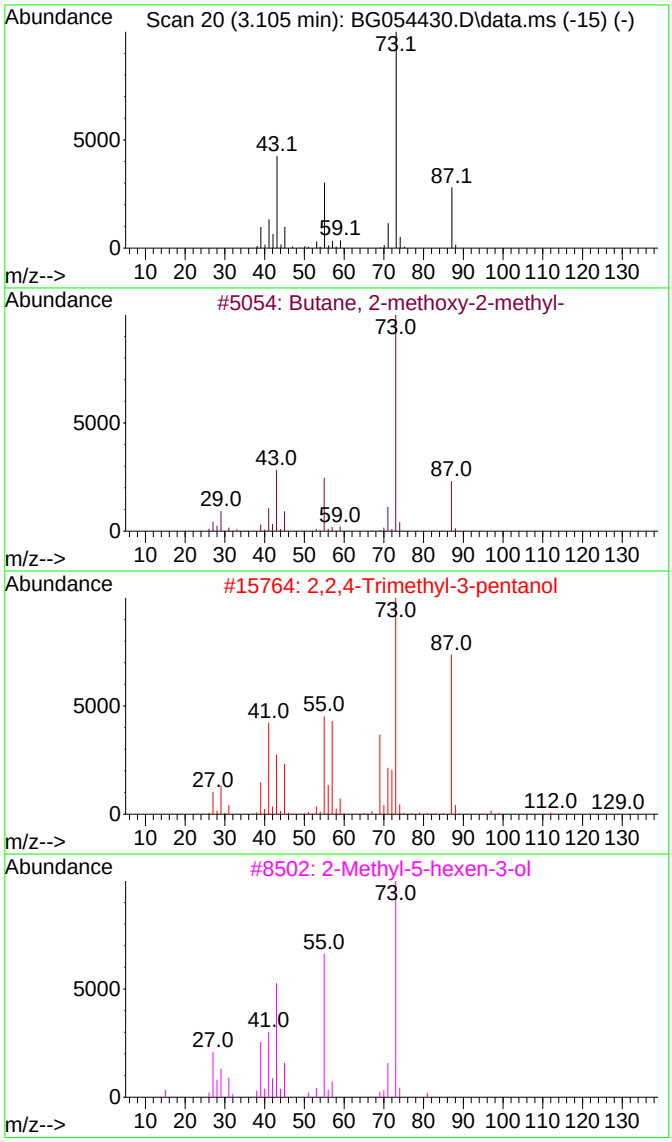
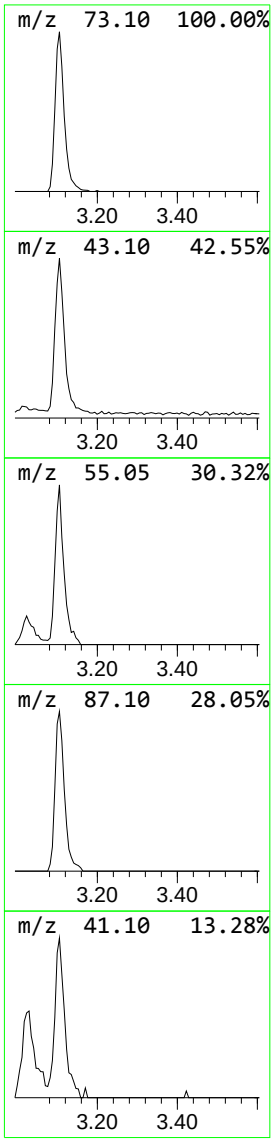
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	24.37 ng	119711	1,4-Dichlorobenzene-d4	7.988

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	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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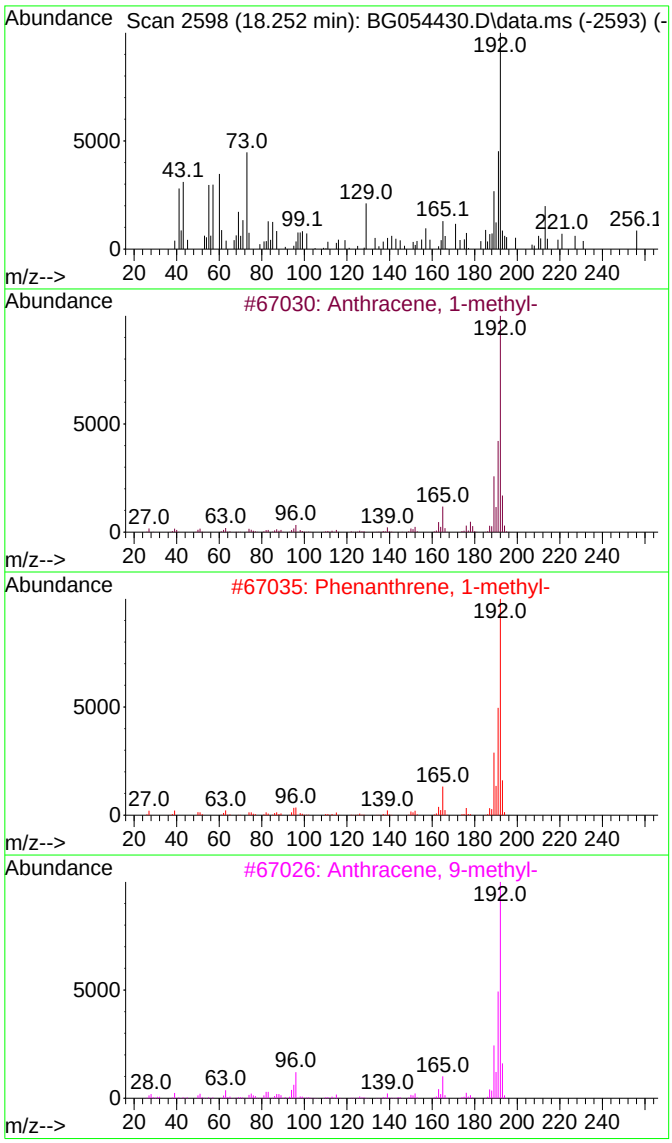
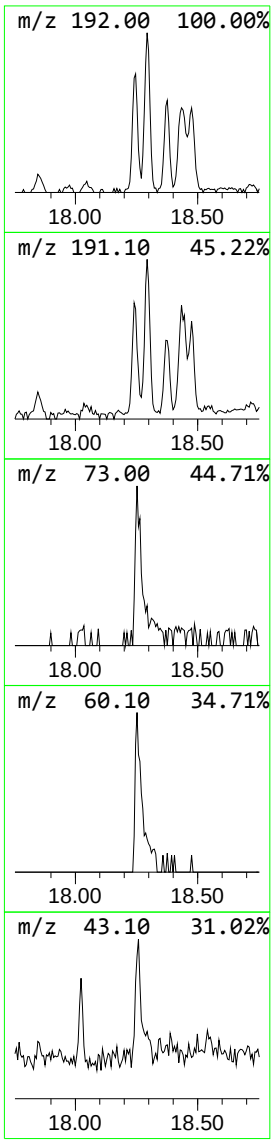
Peak Number 2 unknown18.252 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.252	4.05 ng	59594	Phenanthrene-d10	17.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	49
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	46
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

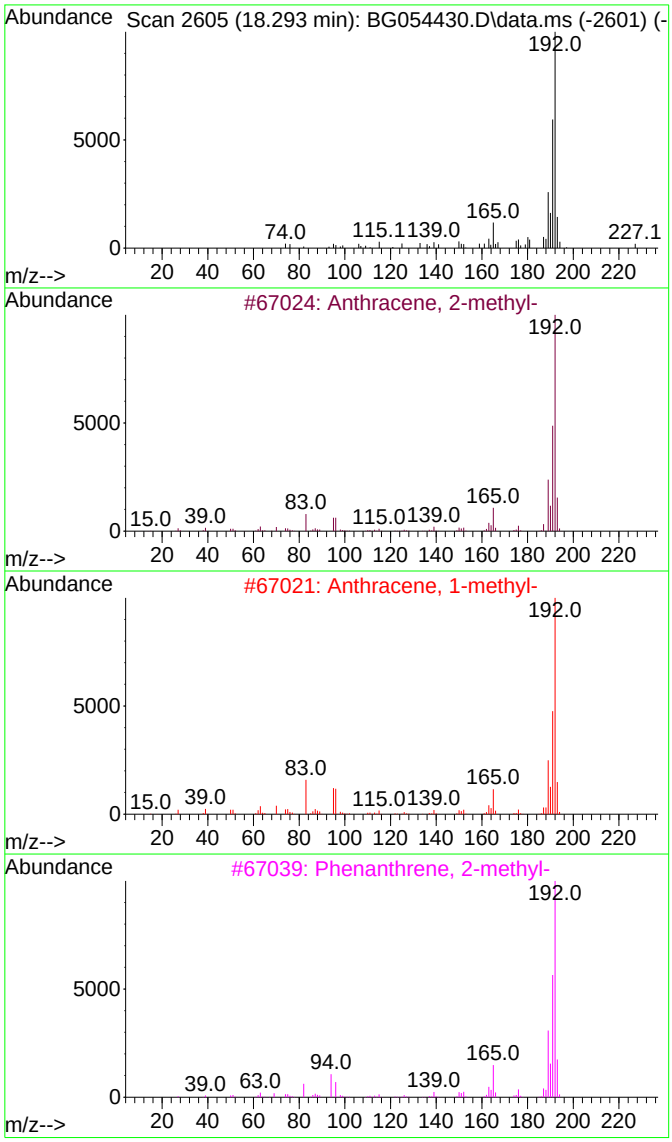
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

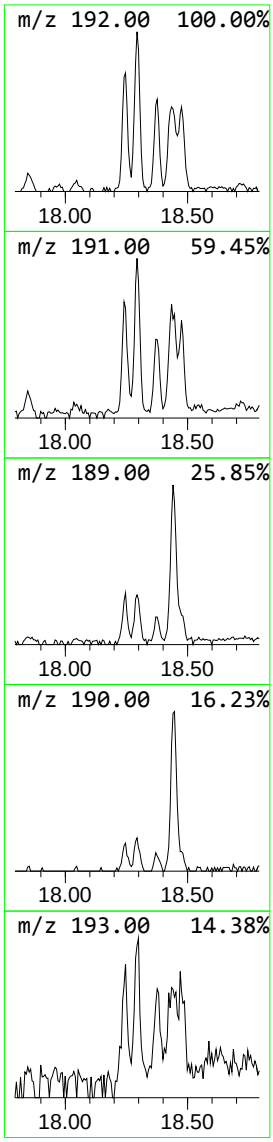
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.293	3.51 ng	51639	Phenanthrene-d10	17.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

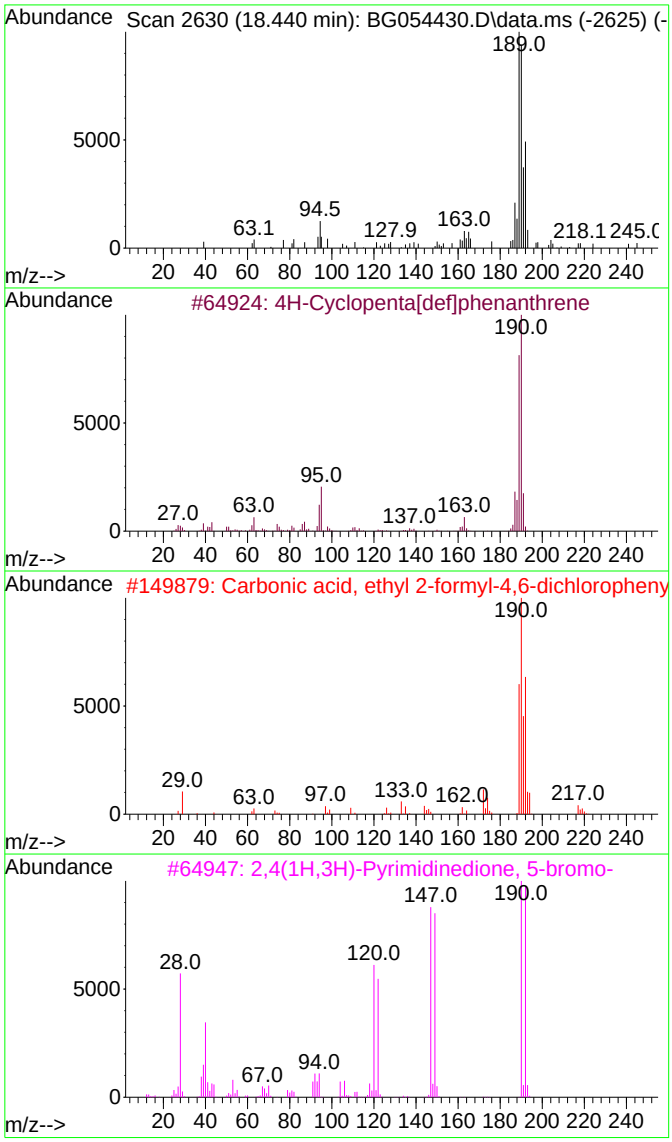
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

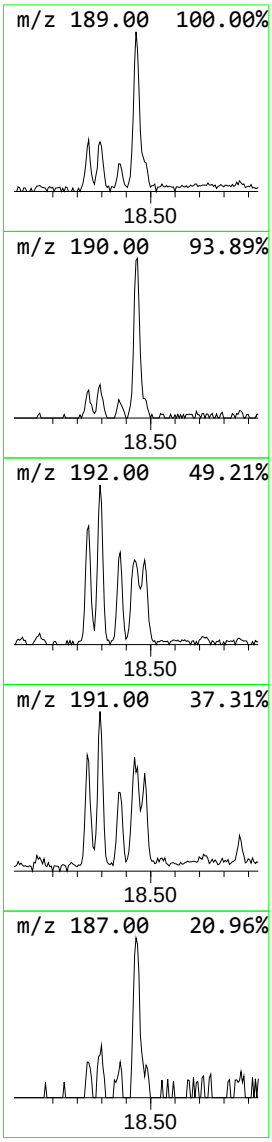
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.440	4.22 ng	62138	Phenanthrene-d10	17.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	38
4	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	35
5	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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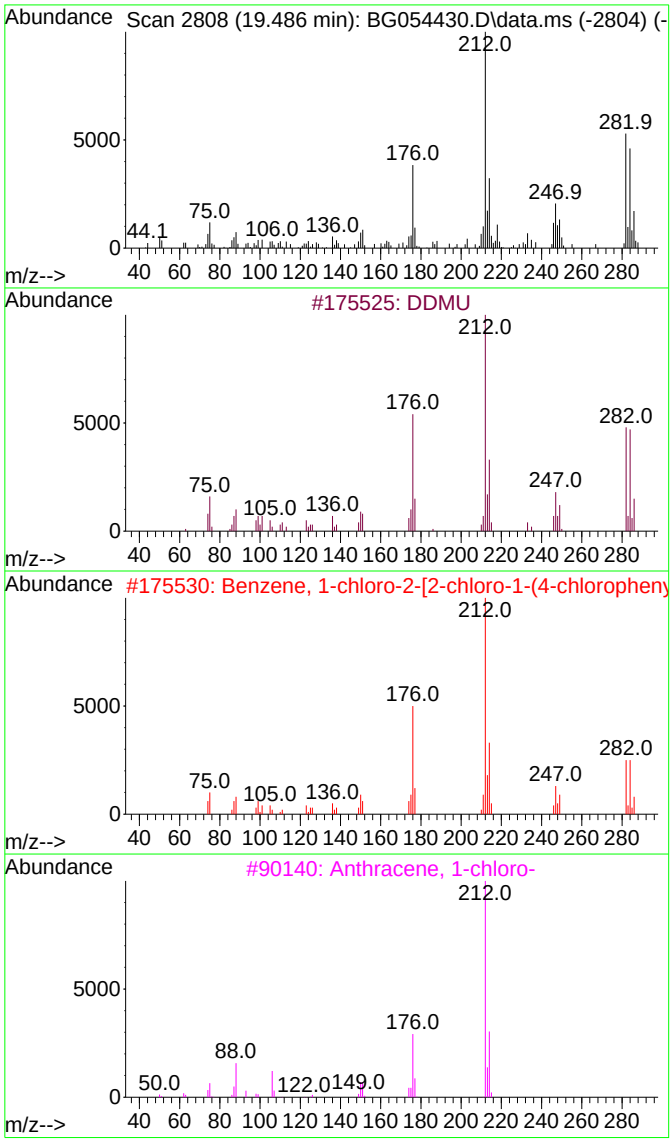
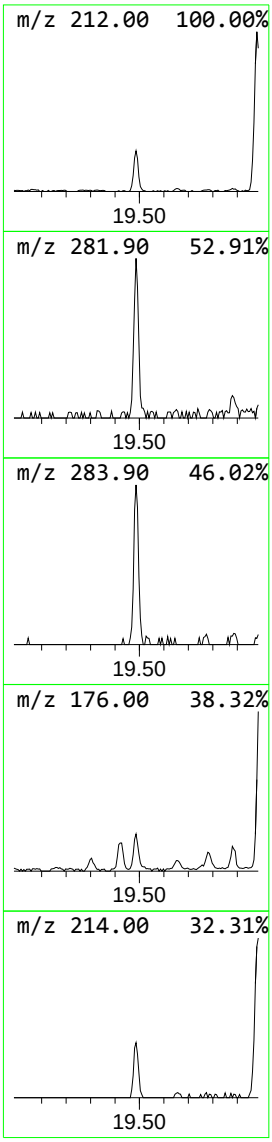
Peak Number 5 DDMU Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	4.90 ng	72112	Phenanthrene-d10	17.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DDMU	282	C14H9Cl3	001022-22-6	98
2	Benzene, 1-chloro-2-[2-chloro-1-...	282	C14H9Cl3	014835-94-0	98
3	Anthracene, 1-chloro-	212	C14H9Cl	004985-70-0	86
4	Anthracene, 2-chloro-	212	C14H9Cl	017135-78-3	64
5	Benzene, 1-chloro-3-(phenylethyn...	212	C14H9Cl	051624-34-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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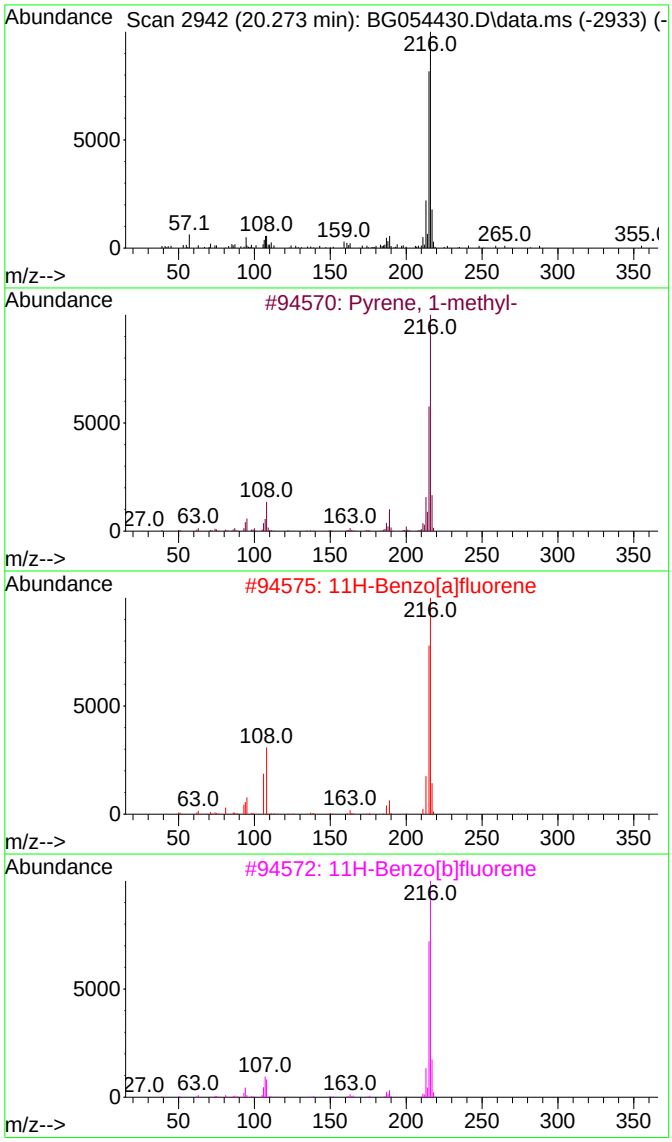
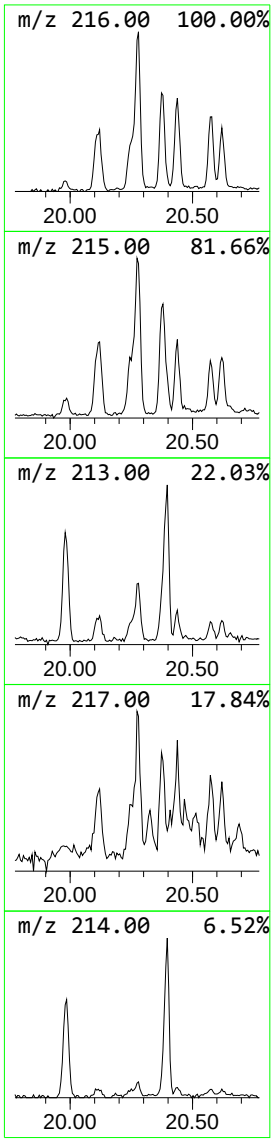
Peak Number 6 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.273	3.17 ng	103969	Chrysene-d12	21.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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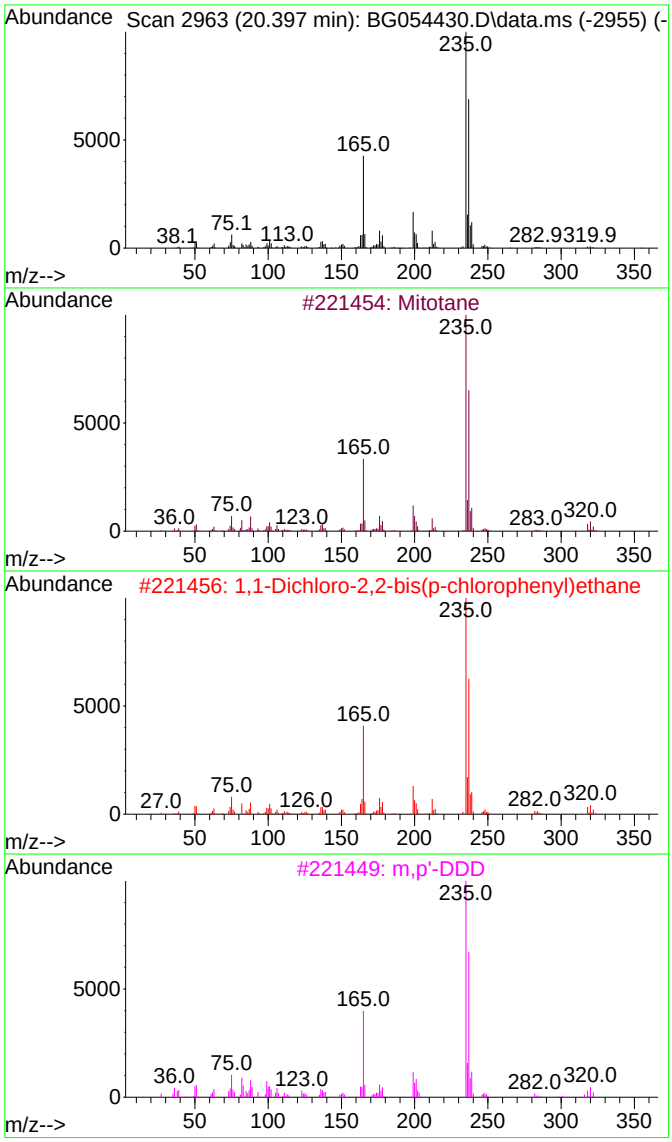
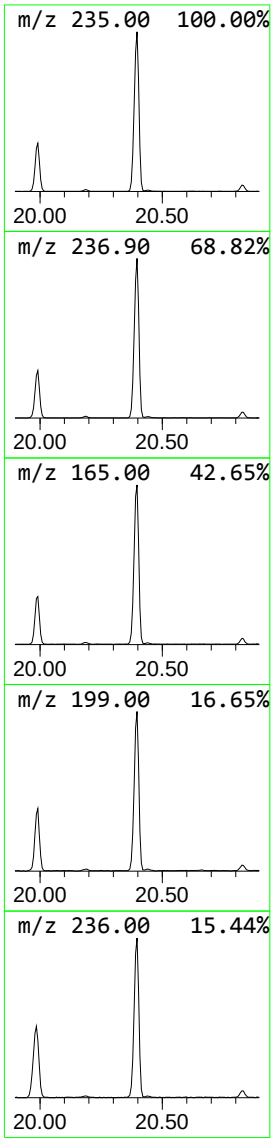
Peak Number 7 Mitotane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.397	85.08 ng	2790830	Chrysene-d12	21.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mitotane	318	C14H10Cl4	000053-19-0	99
2	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	95
3	m,p'-DDD	318	C14H10Cl4	004329-12-8	91
4	3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	91
5	2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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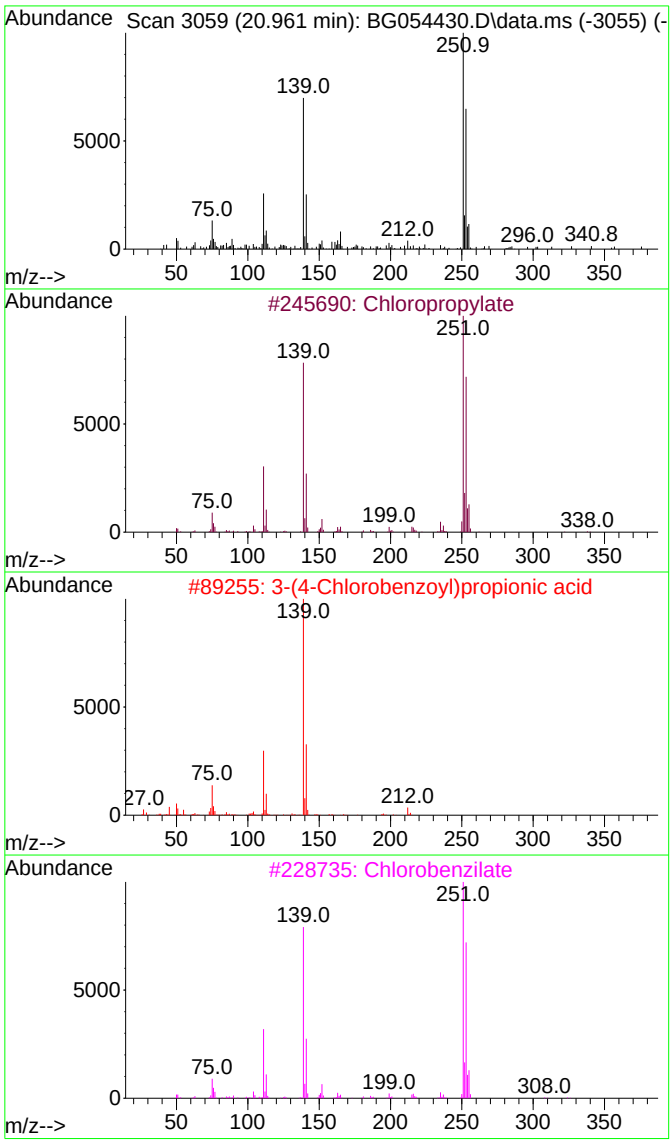
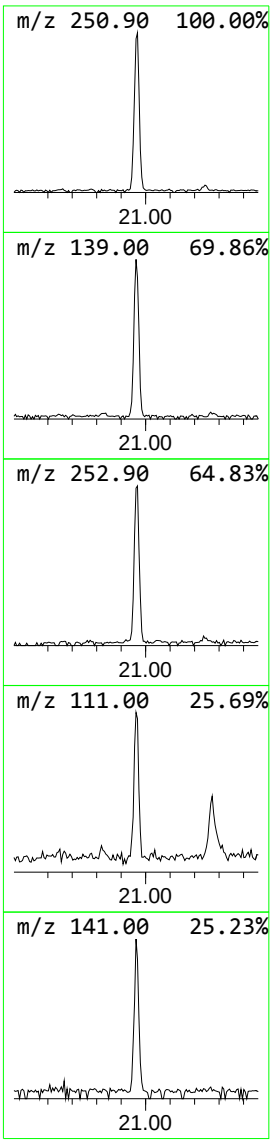
Peak Number 9 Chloropropylate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.961	3.80 ng	124812	Chrysene-d12	21.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloropropylate	338	C17H16Cl2O3	005836-10-2	91
2	3-(4-Chlorobenzoyl)propionic acid	212	C10H9ClO3	003984-34-7	74
3	Chlorobenzilate	324	C16H14Cl2O3	000510-15-6	74
4	Benzamide, 4-chloro-N-(4-methylt...	252	C11H9ClN2OS	339283-30-6	49
5	3-Chlorobenzoic acid, 2,3-dichlo...	300	C13H7Cl3O2	1000357-40-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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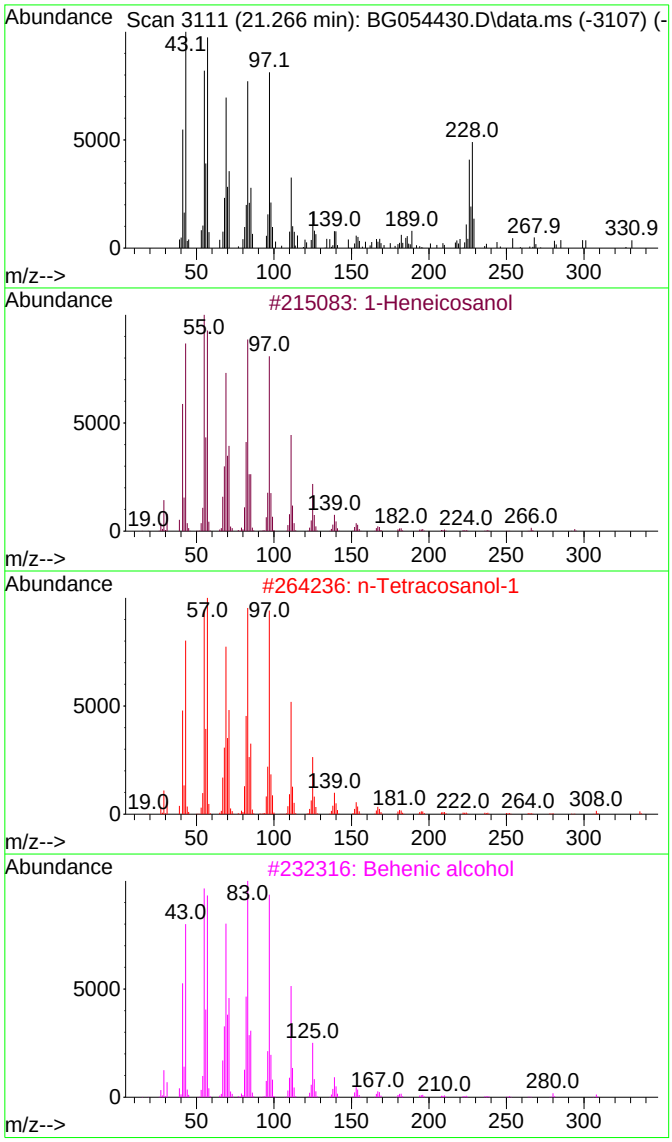
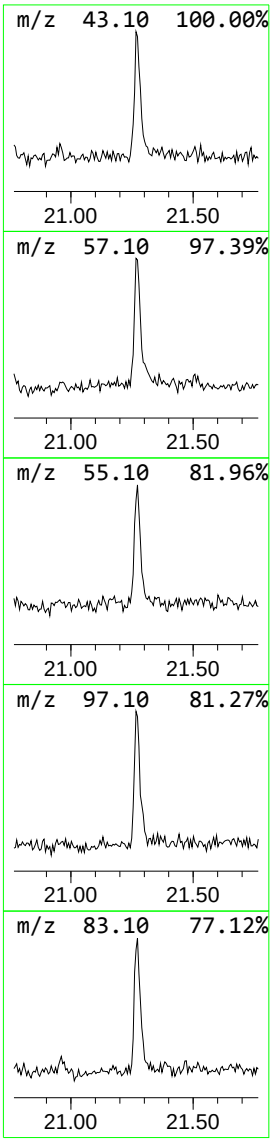
Peak Number 10 1-Heneicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.266	2.07 ng	67864	Chrysene-d12	21.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	83
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	64
3	Behenic alcohol	326	C22H46O	000661-19-8	64
4	1-Docosene	308	C22H44	001599-67-3	64
5	Octacosanol	410	C28H58O	000557-61-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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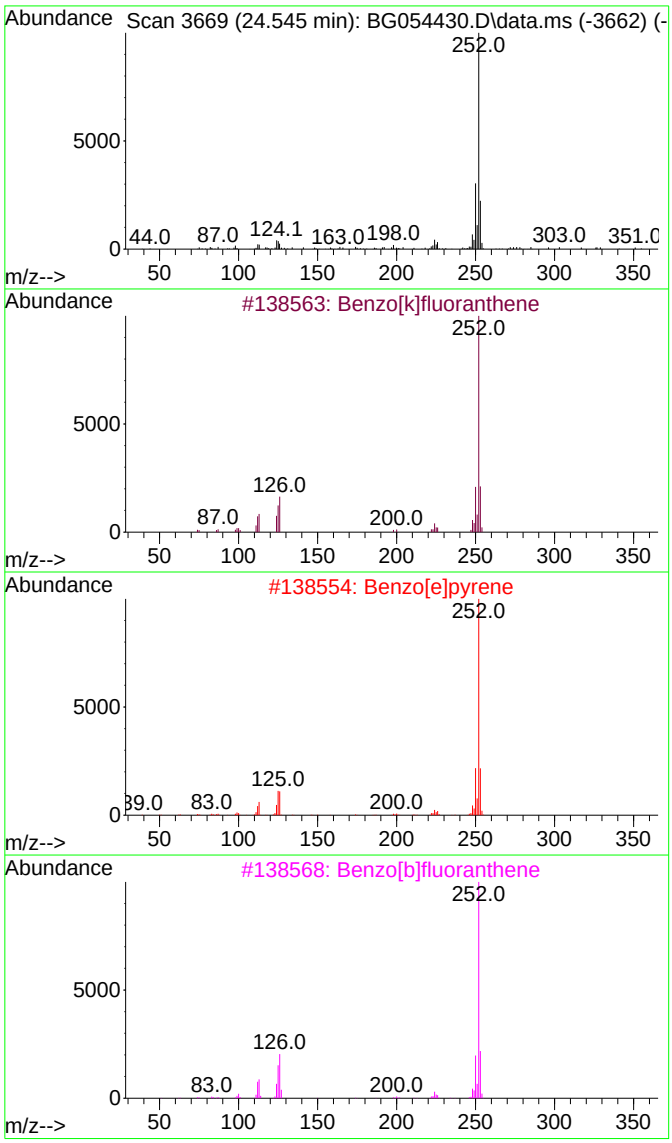
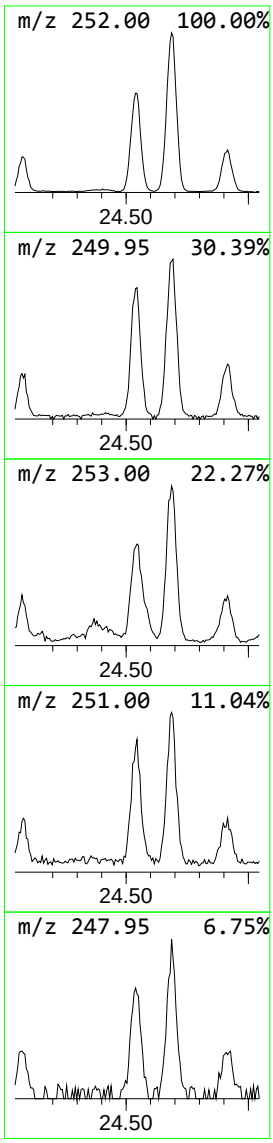
Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.545	12.08 ng	196023	Perylene-d12	24.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
2	Benzo[e]pyrene	252	C20H12	000192-97-2	87
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	87
4	Benzo[a]pyrene	252	C20H12	000050-32-8	87
5	Perylene	252	C20H12	000198-55-0	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054430.D
Acq On : 28 Jul 2022 13:41
Operator : CG/JU
Sample : N3893-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RVE-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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...	3.105	24.4	ng	119711	1	7.988	98242	20.0
unknown18.252	18.252	4.0	ng	59594	4	17.371	294201	20.0
Anthracene, 2-m...	18.293	3.5	ng	51639	4	17.371	294201	20.0
4H-Cyclopenta[d...	18.440	4.2	ng	62138	4	17.371	294201	20.0
DDMU	19.486	4.9	ng	72112	4	17.371	294201	20.0
Pyrene, 1-methyl-	20.273	3.2	ng	103969	5	21.636	656081	20.0
Mitotane	20.397	85.1	ng	2790830	5	21.636	656081	20.0
Chloropropylate	20.961	3.8	ng	124812	5	21.636	656081	20.0
1-Heneicosanol	21.266	2.1	ng	67864	5	21.636	656081	20.0
Benzo[e]pyrene	24.545	12.1	ng	196023	6	24.839	324475	20.0