LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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: BG055582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.337	3	8	14	rBV	338637	589371	20.34%	2.394%
2	3.889	97	102	111	rBV	26327	46300	1.60%	0.188%
3	5.335	342	348	358	rBV	187105	308228	10.64%	1.252%
4	5.805	421	428	440	rBV	1007187	1697250	58.56%	6.894%
5	7.409	693	701	714	rBV	1012601	1831679	63.20%	7.440%
6	8.278	841	849	855	rBV	235608	418325	14.43%	1.699%
7	9.448	1038	1048	1057	rBV	628690	1124434	38.80%	4.567%
8	11.104	1322	1330	1337	rBV	323257	585661	20.21%	2.379%
9	13.519	1734	1741	1749	rVB	1591146	2418414	83.45%	9.823%
10	14.894	1964	1975	1981	rBV	498107	785002	27.09%	3.189%
11	14.959	1981	1986	1992	rVB	37171	58668	2.02%	0.238%
12	15.282	2035	2041	2045	rBV3	20273	39705	1.37%	0.161%
13	15.928	2147	2151	2158	rVB	44390	72652	2.51%	0.295%
14	16.369	2220	2226	2236	rBV	1250299	1907111	65.80%	7.746%
15	16.598	2262	2265	2269	rVB2	28802	37083	1.28%	0.151%
16	16.933	2314	2322	2327	rBV4	11707	29512	1.02%	0.120%
17	17.362	2390	2395	2400	rBV4	21515	42467	1.47%	0.172%
18	17.450	2407	2410	2416	rVB	24787	36138	1.25%	0.147%
19	17.632	2434	2441	2445	rBV	562584	896838	30.95%	3.643%
20	17.673	2445	2448	2455	rVV	464777	663819	22.90%	2.696%
21	17.767	2458	2464	2469	rVB	137914	217995	7.52%	0.885%
22	18.026	2503	2508	2513	rBV2	29969	40999	1.41%	0.167%
23	18.273	2546	2550	2555	rBV2	25131	37858	1.31%	0.154%
24	18.490	2582	2587	2593	rBV2	164142	284240	9.81%	1.155%
25	18.549	2593	2597	2603	rVB	74414	116792	4.03%	0.474%
26	18.631	2607	2611	2616	rVB	34357	51804	1.79%	0.210%
27	18.701	2617	2623	2627	rBV3	113306	209365	7.22%	0.850%
28	18.989	2668	2672	2677	rBV	51953	77396	2.67%	0.314%
29	19.407	2739	2743	2748	rBV2	28470	45435	1.57%	0.185%
30	19.671	2783	2788	2794	rVB	960589	1327672	45.81%	5.393%
31	19.753	2798	2802	2807	rVV3	74148	110564	3.81%	0.449%
32	20.000	2838	2844	2845	rBV	165233	251927	8.69%	1.023%
33	20.029	2845	2849	2856	rVB	738941	1126424	38.87%	4.575%
34	20.217	2875	2881	2886	rBV	2169743	2898156	100.00%	11.772%
35	20.517	2928	2932	2936	rVB	137101	192947	6.66%	0.784%
36	20.611	2945	2948	2953	rBV	125337	168457	5.81%	0.684%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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	21.539	3102	3106	3110	rVB2	119665	167670	5.79%	0.681%
38	21.927	3164	3172	3178	rBV2	550719	1566220	54.04%	6.362%
39	21.986	3178	3182	3192	rVB	306296	521464	17.99%	2.118%
40	24.266	3564	3570	3578	rBV2	179042	593575	20.48%	2.411%
41	25.206	3723	3730	3746	rVB	165466	515279	17.78%	2.093%
42	25.364	3751	3757	3766	rVV2	175018	508361	17.54%	2.065%

Sum of corrected areas: 24619257

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
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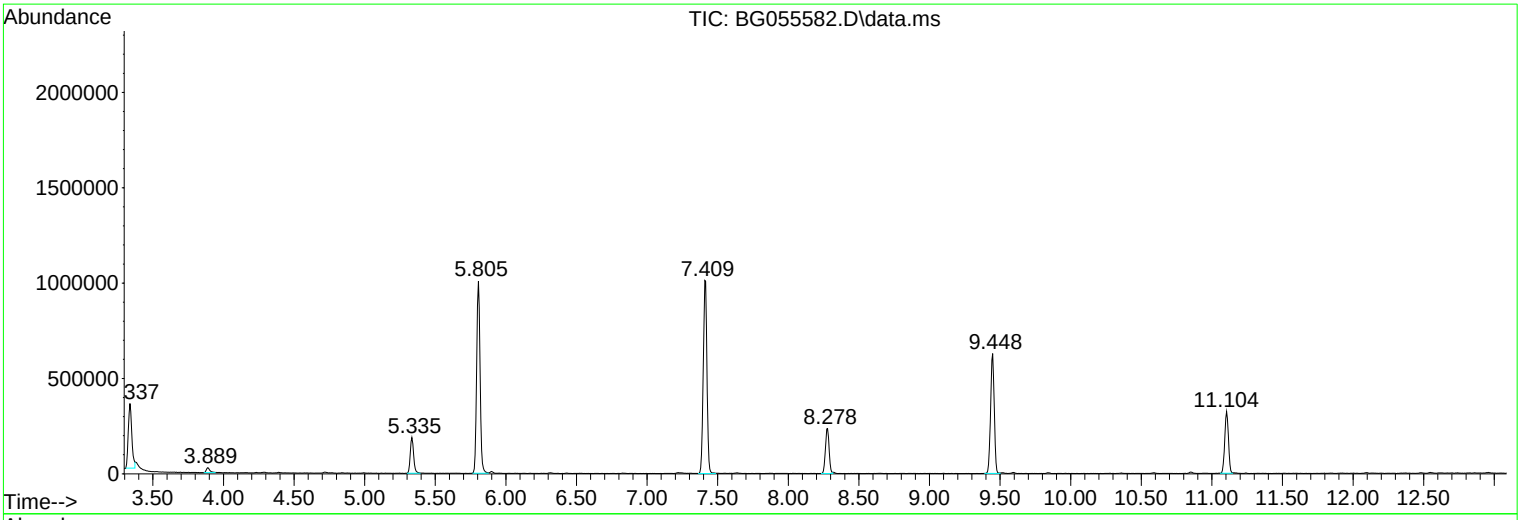
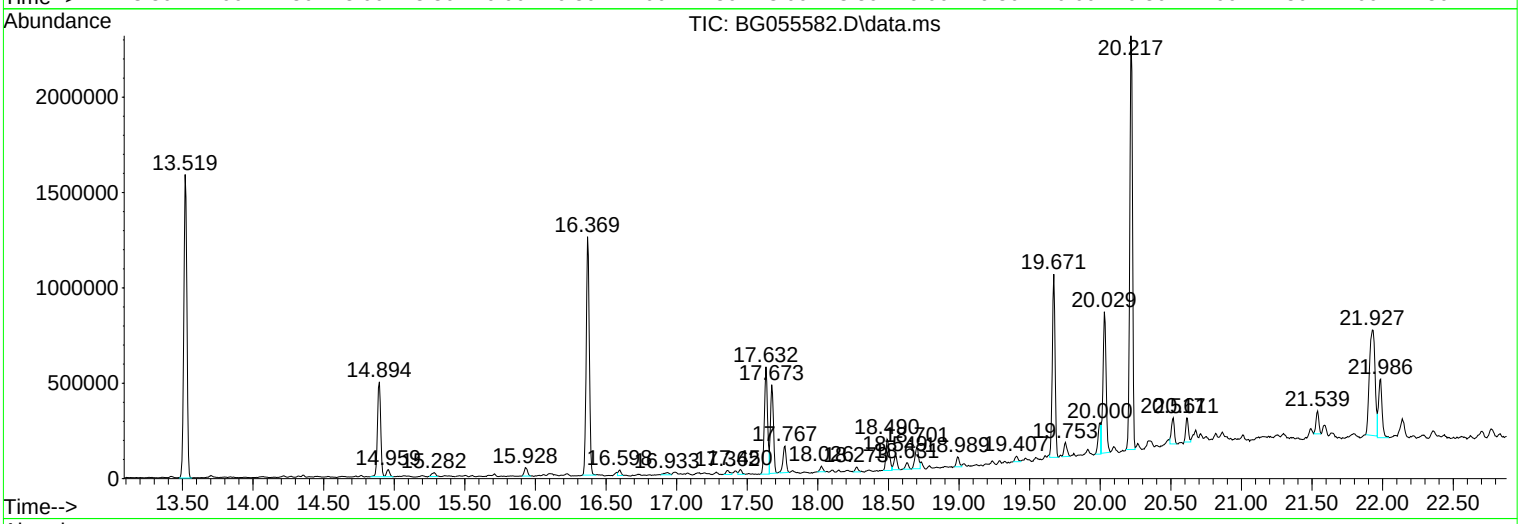
ALS Vial : 15 Sample Multiplier: 1

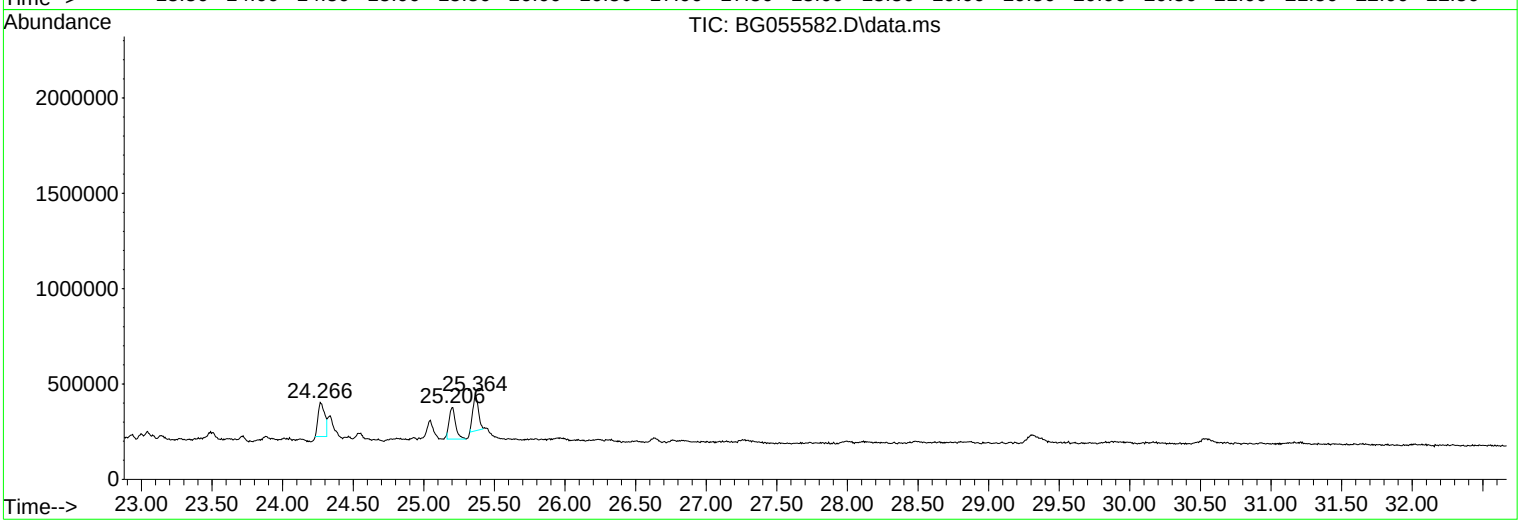
Instrument :
BNA_G
ClientSampleId :
TP-13

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 : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

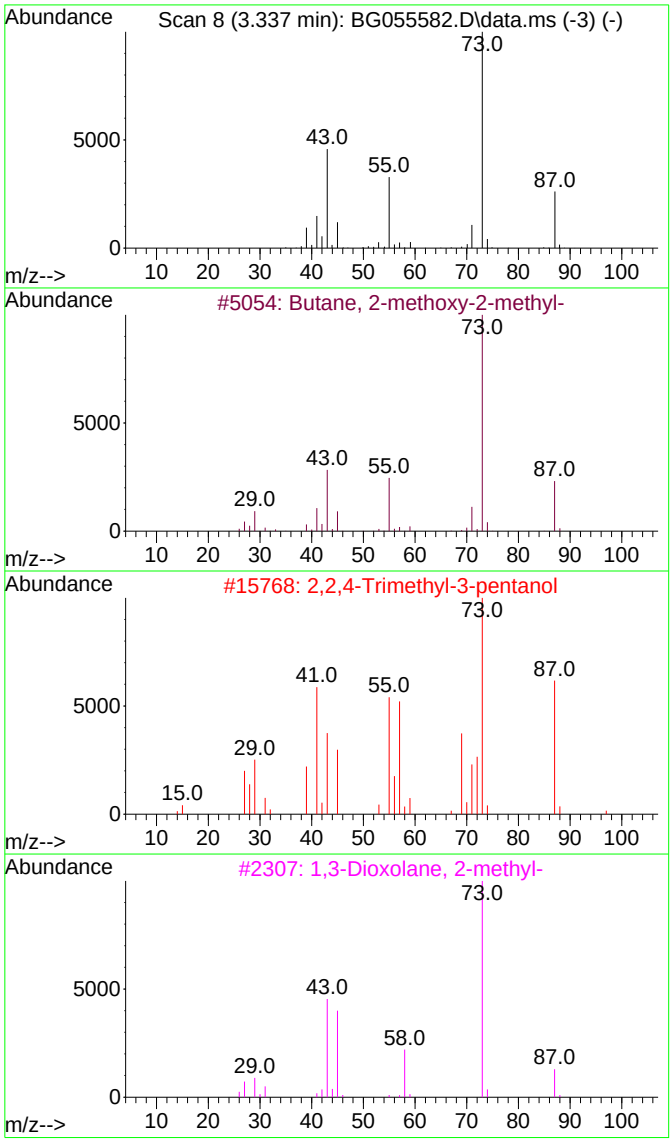
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

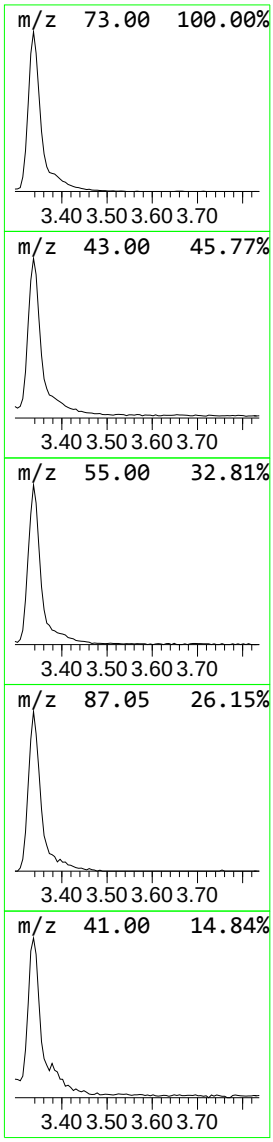
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.337	28.18 ng	589371	1,4-Dichlorobenzene-d4	8.278

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

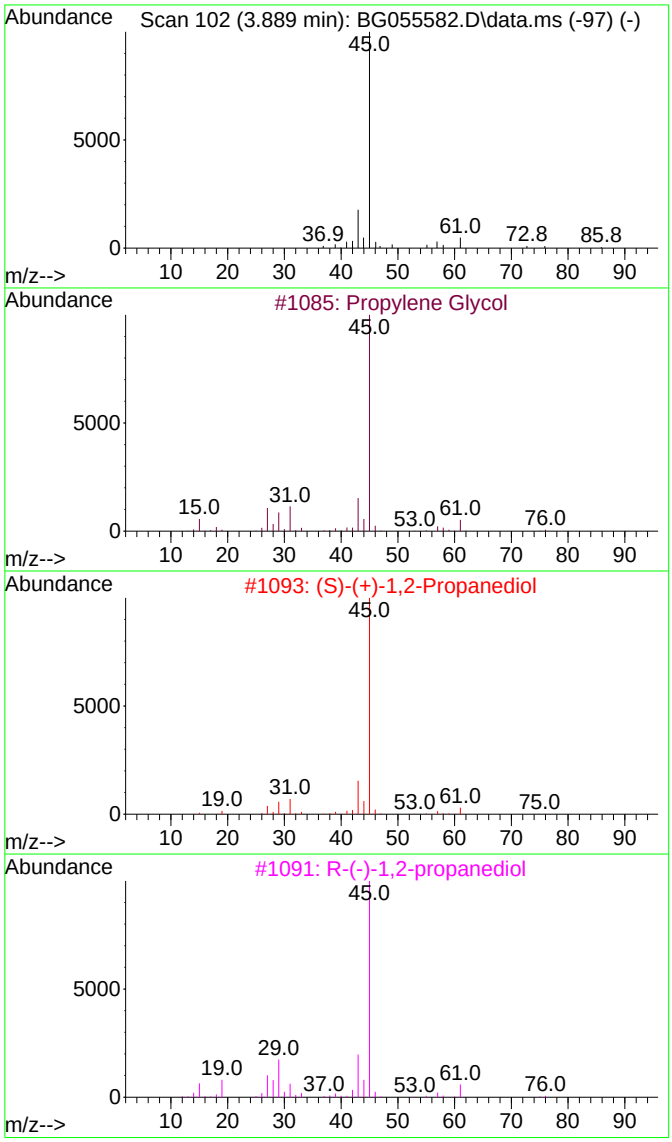
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

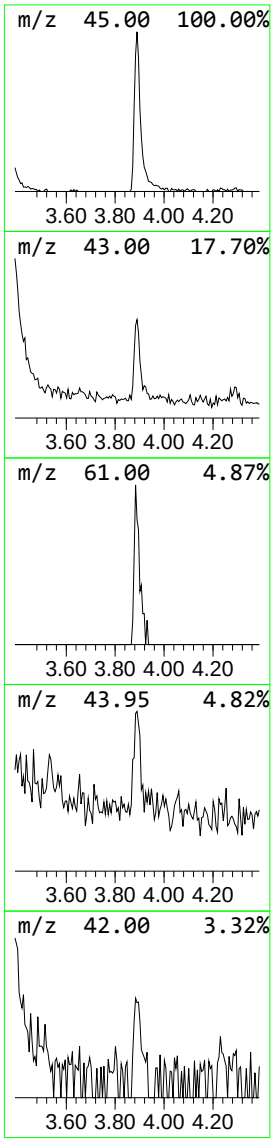
****

Peak Number 2 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.889	2.21 ng	46300	1,4-Dichlorobenzene-d4	8.278

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	72
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Methyltartronic acid	134	C4H6O5	000595-98-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

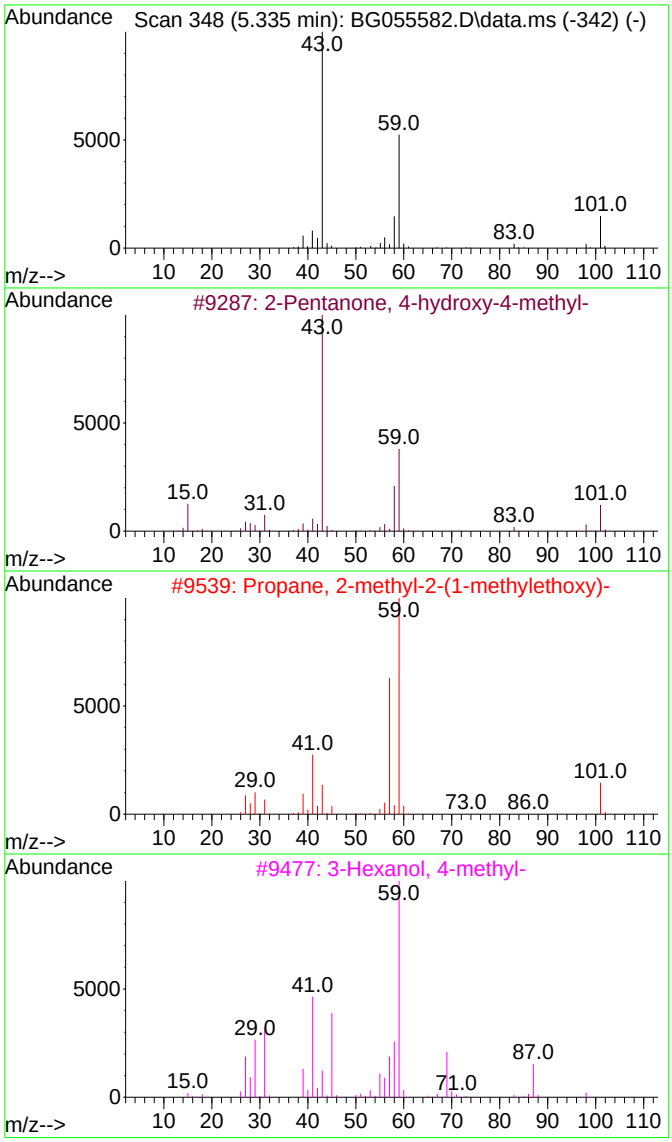
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

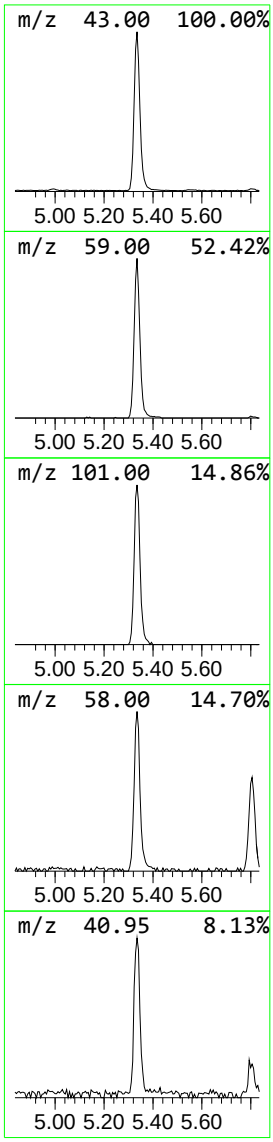
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.335	14.74 ng	308228	1,4-Dichlorobenzene-d4	8.278

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

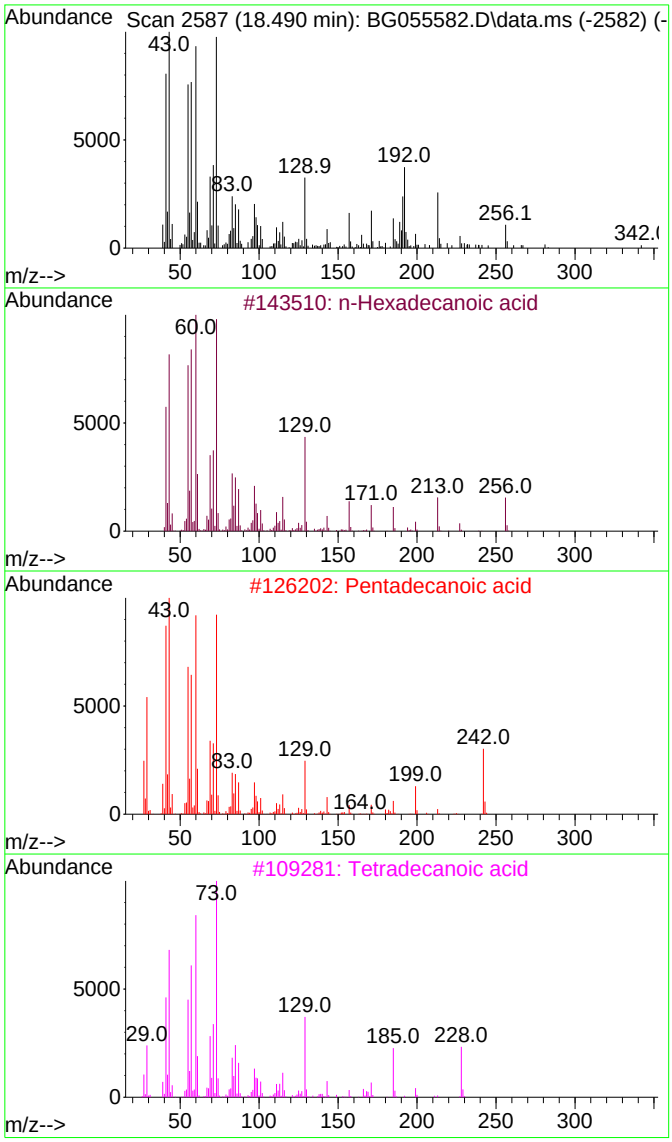
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

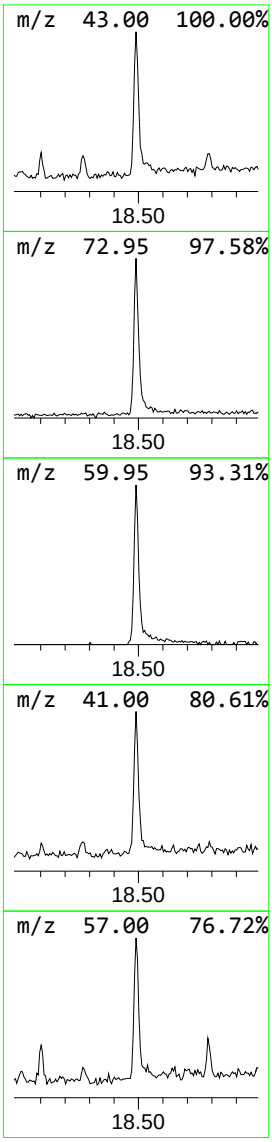
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.490	6.34 ng	284240	Phenanthrene-d10	17.632

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Octadecanoic acid	284	C18H36O2	000057-11-4	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

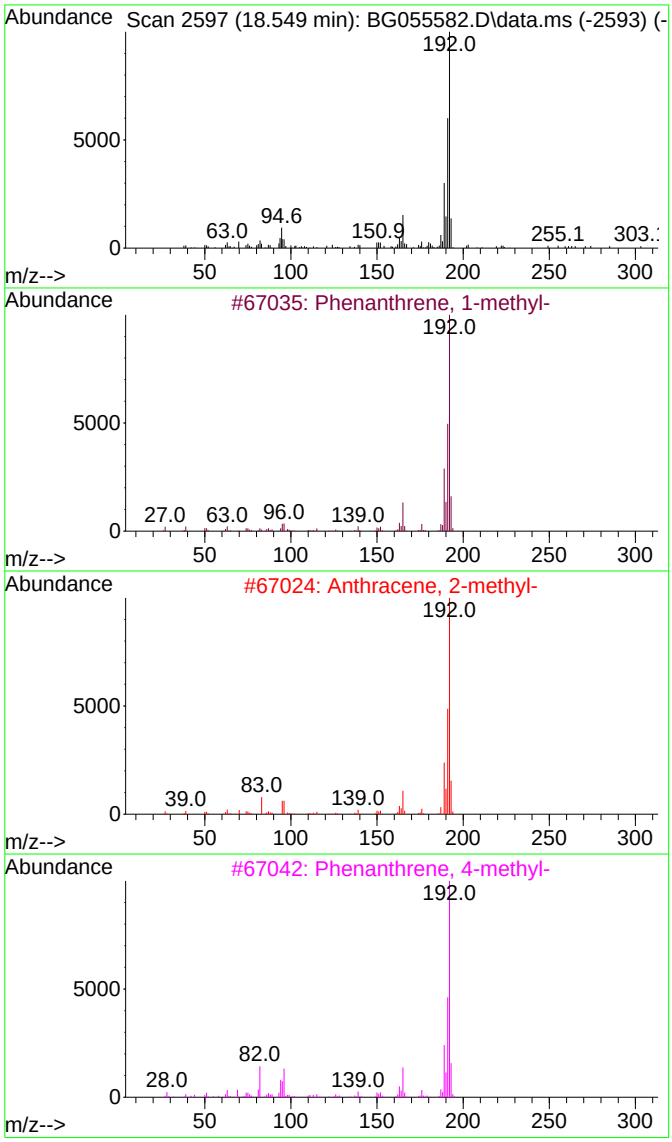
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

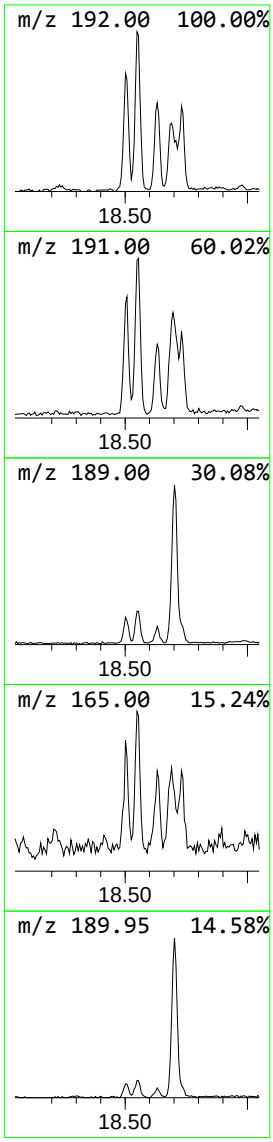
****

Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.549	2.60 ng	116792	Phenanthrene-d10	17.632

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

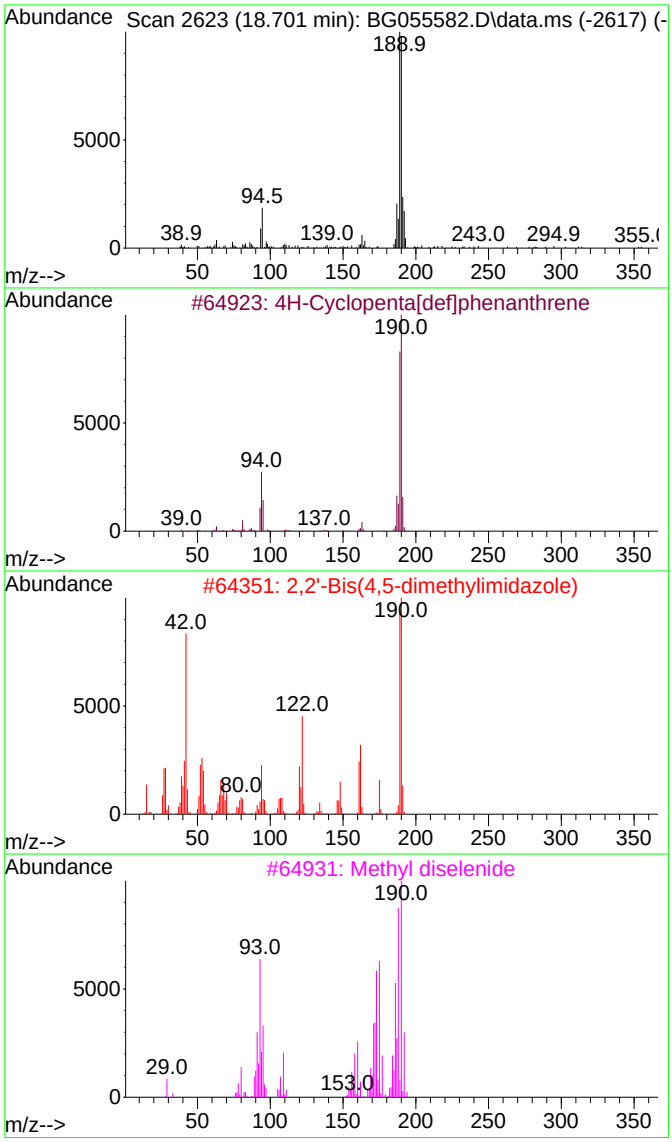
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

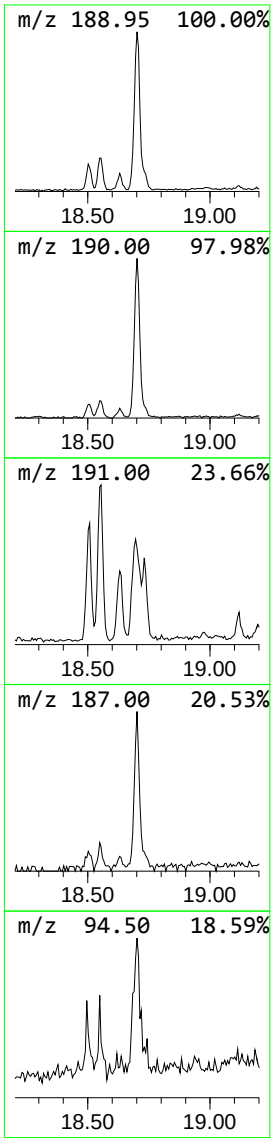
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.701	4.67 ng	209365	Phenanthrene-d10	17.632

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	38
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
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Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

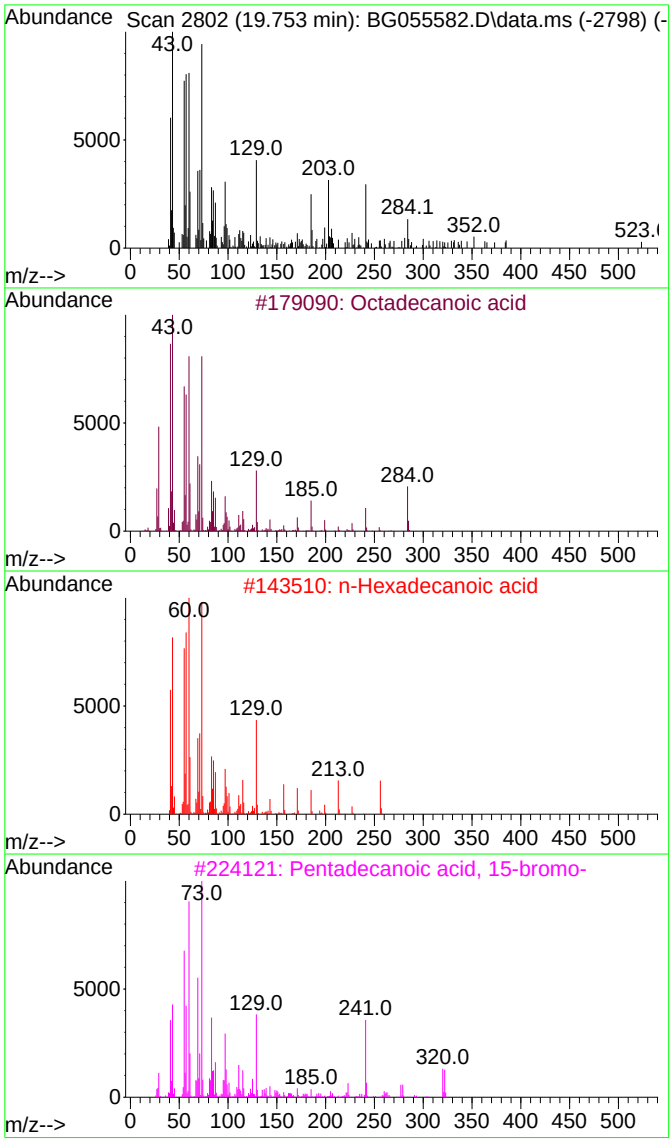
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

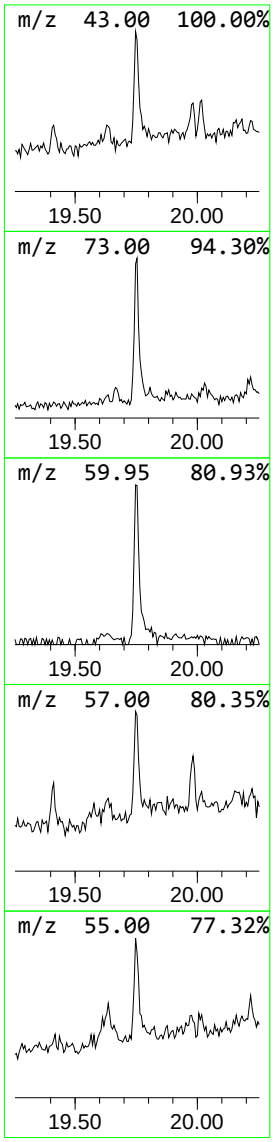
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.753	2.47 ng	110564	Phenanthrene-d10	17.632

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Pentadecanoic acid, 15-bromo-	320	C15H29BrO2	056523-59-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

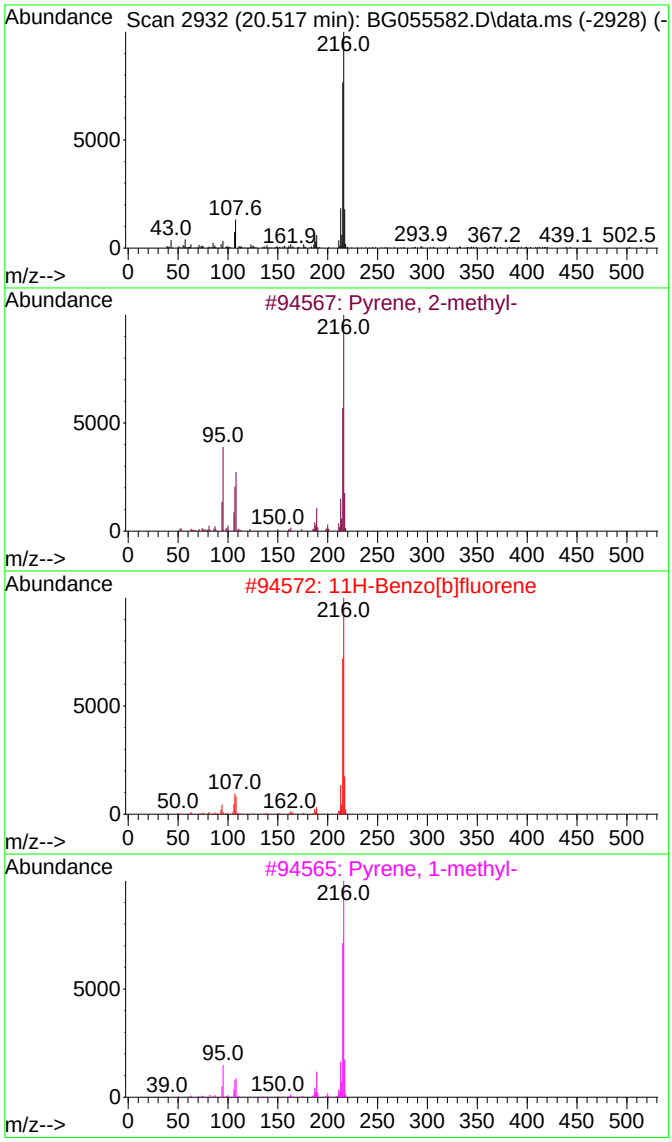
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

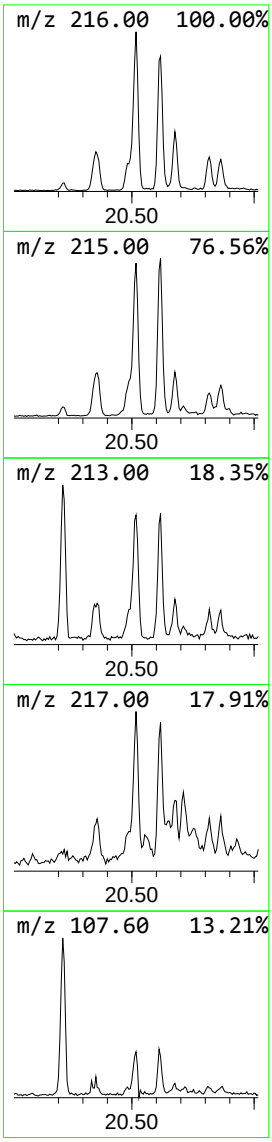
****

Peak Number 8 Pyrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.517	2.46 ng	192947	Chrysene-d12	21.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	83





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Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

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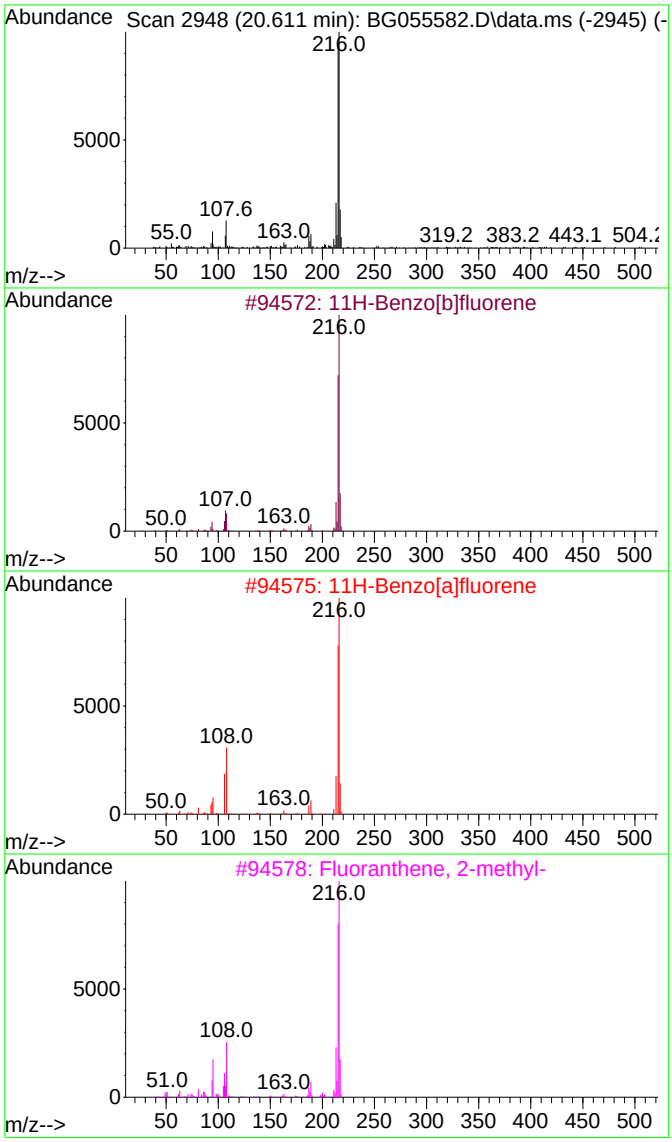
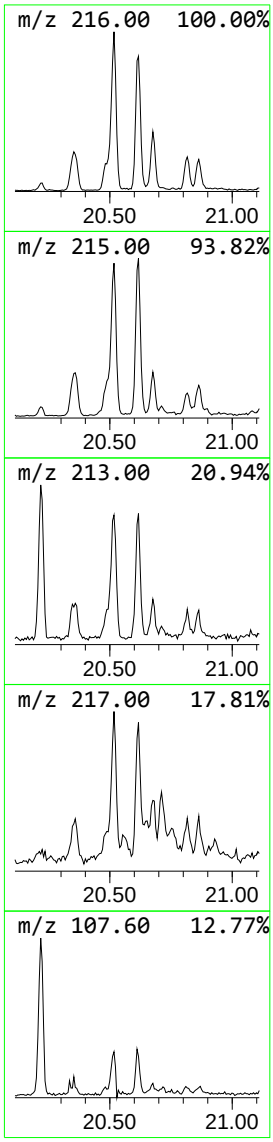
Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.611	2.15 ng	168457	Chrysene-d12	21.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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

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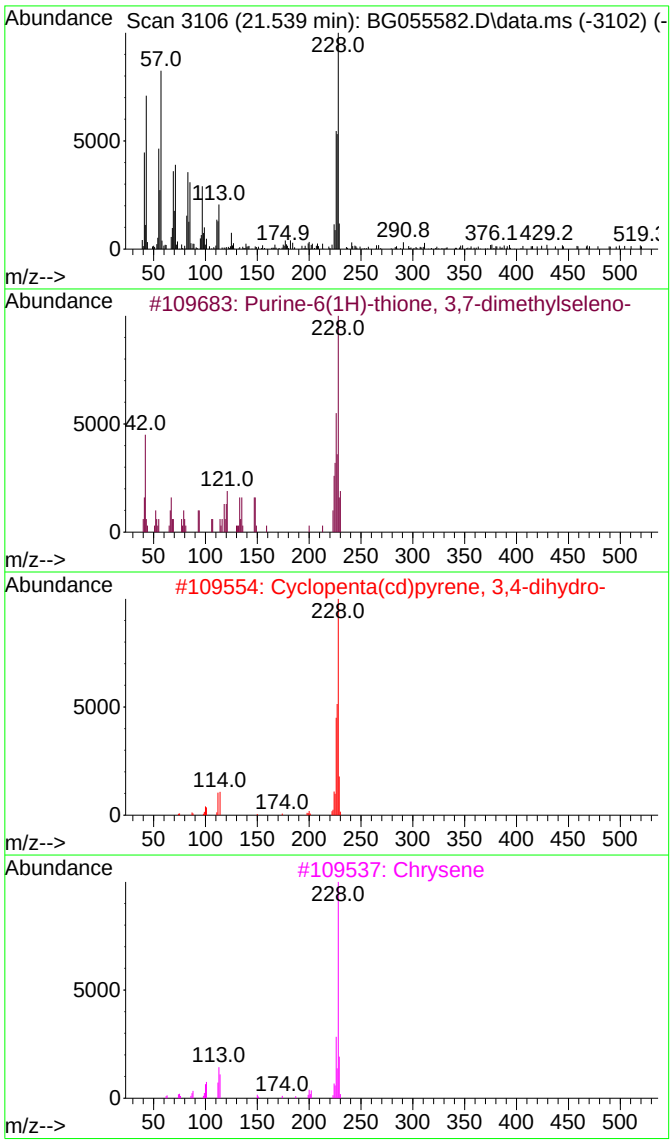
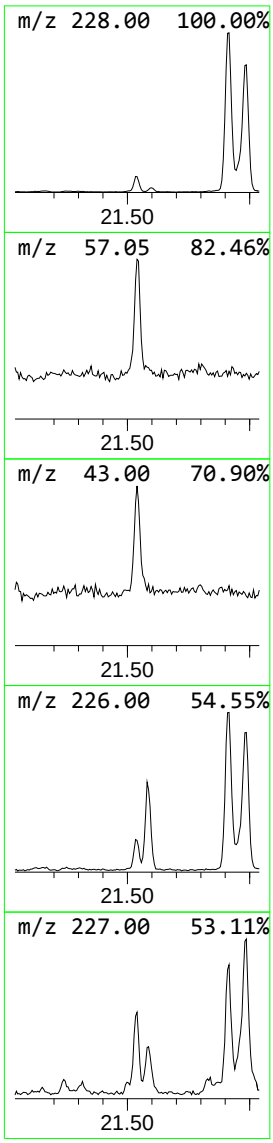
Peak Number 10 unknown21.539 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.539	2.14 ng	167670	Chrysene-d12	21.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	47
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	46
3	Chrysene	228	C18H12	000218-01-9	38
4	Benz[a]anthracene	228	C18H12	000056-55-3	38
5	Benzo[c]phenanthrene	228	C18H12	000195-19-7	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055582.D
Acq On : 12 Nov 2022 1:52
Operator : CG/JU
Sample : N5509-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-13

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...	3.337	28.2	ng	589371	1	8.278	418325	20.0
Propylene Glycol	3.889	2.2	ng	46300	1	8.278	418325	20.0
2-Pentanone, 4-...	5.335	14.7	ng	308228	1	8.278	418325	20.0
n-Hexadecanoic ...	18.490	6.3	ng	284240	4	17.632	896838	20.0
Phenanthrene, 1...	18.549	2.6	ng	116792	4	17.632	896838	20.0
4H-Cyclopenta[d...	18.701	4.7	ng	209365	4	17.632	896838	20.0
Octadecanoic acid	19.753	2.5	ng	110564	4	17.632	896838	20.0
Pyrene, 2-methyl-	20.517	2.5	ng	192947	5	21.933	1566220	20.0
11H-Benzo[b]flu...	20.611	2.1	ng	168457	5	21.933	1566220	20.0
unknown21.539	21.539	2.1	ng	167670	5	21.933	1566220	20.0