LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

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-BG041724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	25	30	35	rBV	27187	39848	1.99%	0.316%
2	3.675	113	117	124	rBV	21526	29809	1.49%	0.236%
3	5.526	426	432	439	rBV	408630	630401	31.48%	4.992%
4	7.106	694	701	709	rBV	439542	738813	36.89%	5.850%
5	7.941	836	843	849	rBB	109183	176099	8.79%	1.394%
6	9.092	1031	1039	1049	rBV	287005	504598	25.19%	3.996%
7	10.732	1310	1318	1325	rBV	138242	241971	12.08%	1.916%
8	13.193	1730	1737	1744	rBV	737185	1147802	57.31%	9.089%
9	14.568	1961	1971	1977	rBV	256243	392361	19.59%	3.107%
10	16.055	2217	2224	2232	rBV	812195	1202967	60.07%	9.526%
11	16.719	2332	2337	2344	rBV2	32605	45179	2.26%	0.358%
12	17.312	2430	2438	2442	rBV	325860	508818	25.41%	4.029%
13	17.353	2442	2445	2452	rVB	84529	124409	6.21%	0.985%
14	17.488	2464	2468	2474	rVB6	21586	30947	1.55%	0.245%
15	17.712	2501	2506	2512	rBV	12282	21522	1.07%	0.170%
16	18.088	2566	2570	2578	rBV2	39555	56847	2.84%	0.450%
17	18.223	2583	2593	2602	rBV2	228569	368130	18.38%	2.915%
18	18.387	2615	2621	2624	rBV4	17998	30569	1.53%	0.242%
19	18.587	2650	2655	2660	rBV9	15285	28308	1.41%	0.224%
20	18.722	2676	2678	2682	rVB2	18783	22476	1.12%	0.178%
21	19.245	2763	2767	2771	rVB4	15486	22162	1.11%	0.175%
22	19.369	2782	2788	2796	rVB	256397	366979	18.32%	2.906%
23	19.492	2805	2809	2816	rVB	61040	86906	4.34%	0.688%
24	19.727	2845	2849	2856	rVB	191768	286560	14.31%	2.269%
25	19.803	2858	2862	2868	rVB5	14933	28383	1.42%	0.225%
26	19.938	2876	2885	2890	rBV	1499513	2002772	100.00%	15.859%
27	20.056	2899	2905	2910	rBV4	17040	46934	2.34%	0.372%
28	20.226	2930	2934	2938	rVB	37663	54207	2.71%	0.429%
29	20.320	2946	2950	2954	rBV	32089	46156	2.30%	0.365%
30	20.379	2955	2960	2964	rBV2	33426	55806	2.79%	0.442%
31	20.520	2980	2984	2987	rBV2	20208	24678	1.23%	0.195%
32	20.567	2989	2992	2996	rVB4	14906	22888	1.14%	0.181%
33	20.978	3058	3062	3067	rVB	31764	51322	2.56%	0.406%
34	21.137	3084	3089	3090	rBV3	23002	30417	1.52%	0.241%
35	21.161	3090	3093	3097	rVV	34550	55704	2.78%	0.441%
36	21.202	3097	3100	3103	rVV2	25591	37259	1.86%	0.295%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

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-BG041724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.249	3103	3108	3114	rVV3	70215	133372	6.66%	1.056%
38	21.302	3114	3117	3127	rVB2	26751	51082	2.55%	0.404%
39	21.484	3144	3148	3152	rBV6	14141	22405	1.12%	0.177%
40	21.572	3154	3163	3167	rVV2	384117	805703	40.23%	6.380%
41	21.613	3167	3170	3178	rVB	128705	215675	10.77%	1.708%
42	21.713	3183	3187	3192	rBV6	15263	29736	1.48%	0.235%
43	21.766	3192	3196	3198	rBV3	16945	24215	1.21%	0.192%
44	21.965	3227	3230	3238	rVB5	21091	32404	1.62%	0.257%
45	22.353	3292	3296	3302	rBV4	31241	53452	2.67%	0.423%
46	22.588	3334	3336	3342	rVV6	14704	26541	1.33%	0.210%
47	22.747	3359	3363	3368	rBV3	32627	53632	2.68%	0.425%
48	23.252	3443	3449	3459	rVB	173694	343879	17.17%	2.723%
49	23.705	3519	3526	3533	rBV	85443	261135	13.04%	2.068%
50	24.398	3639	3644	3653	rVB	52862	127255	6.35%	1.008%
51	24.539	3662	3668	3678	rVB2	62276	175615	8.77%	1.391%
52	24.692	3684	3694	3702	rBV	225963	617523	30.83%	4.890%
53	28.229	4287	4296	4298	rBV4	21676	64506	3.22%	0.511%
54	29.304	4473	4479	4480	rBV6	17956	29394	1.47%	0.233%

Sum of corrected areas: 12628531

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
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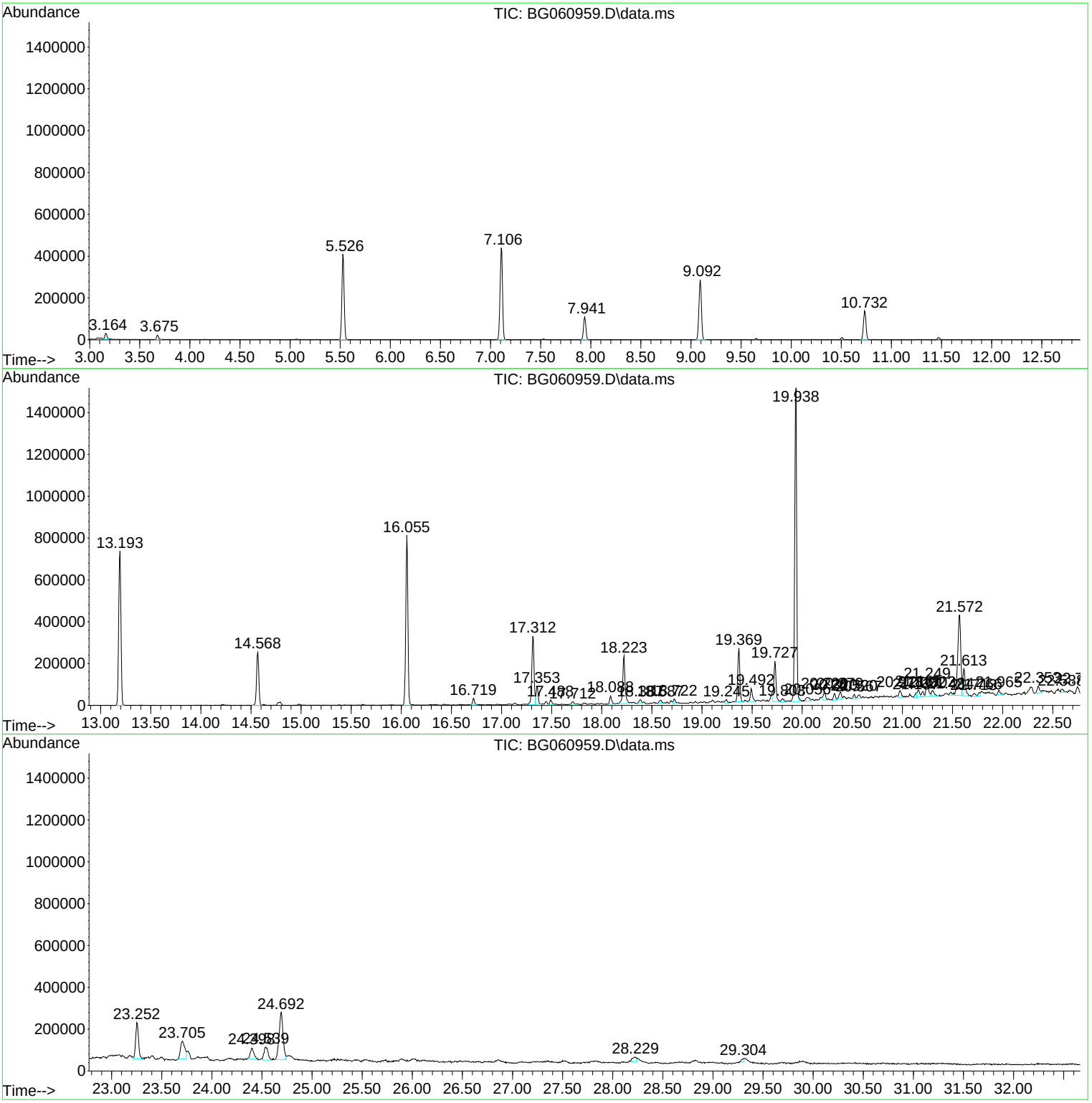
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

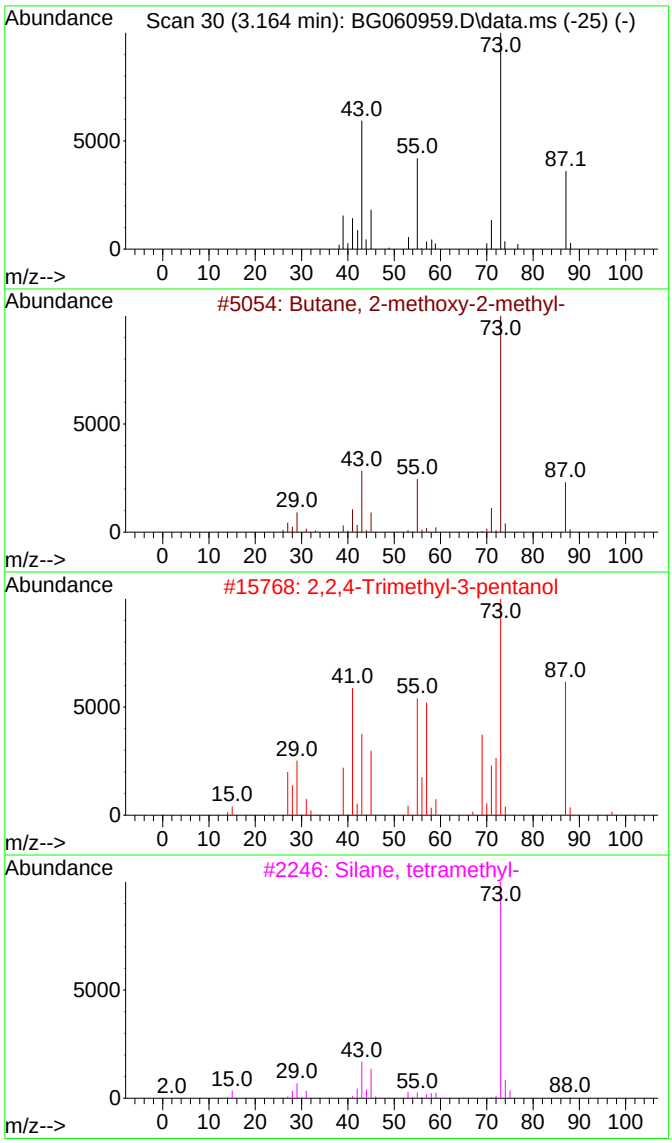
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

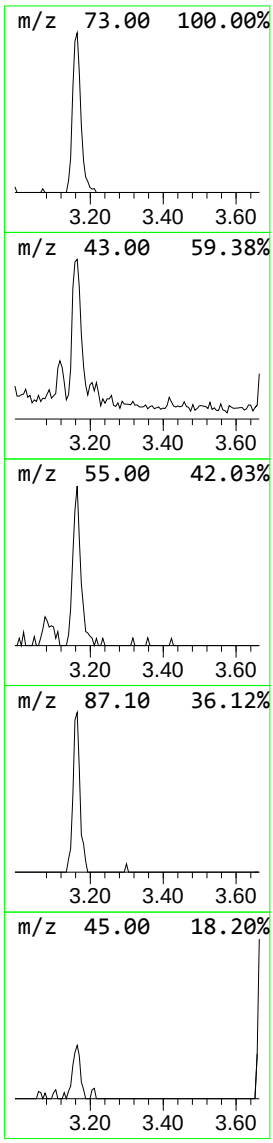
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	4.53 ng	39848	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

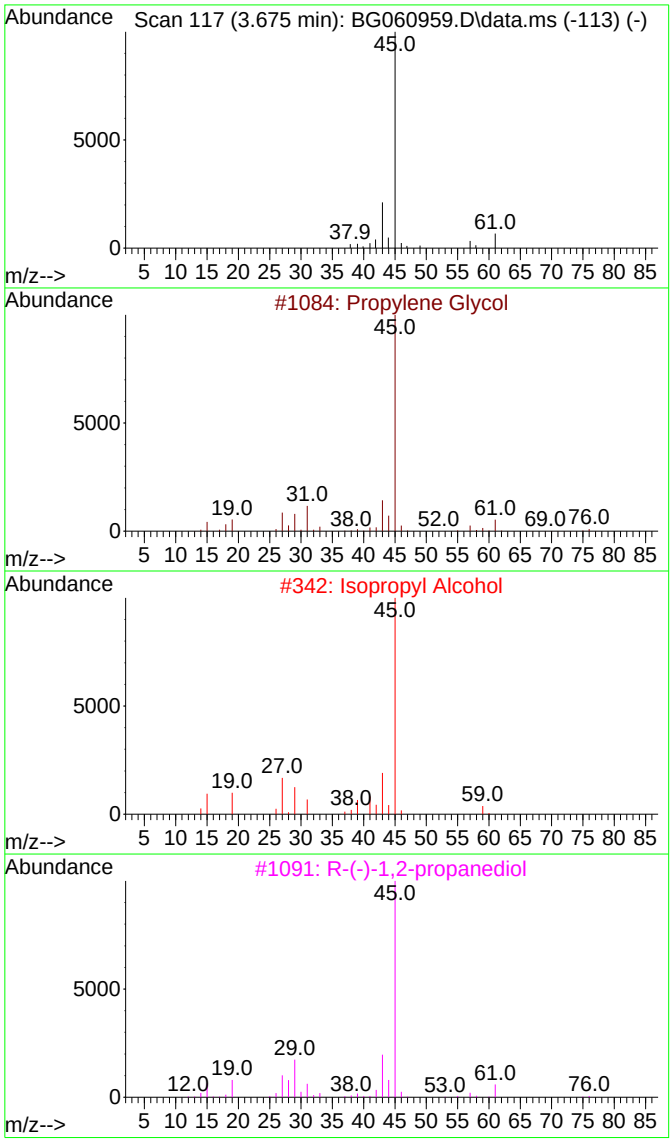
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

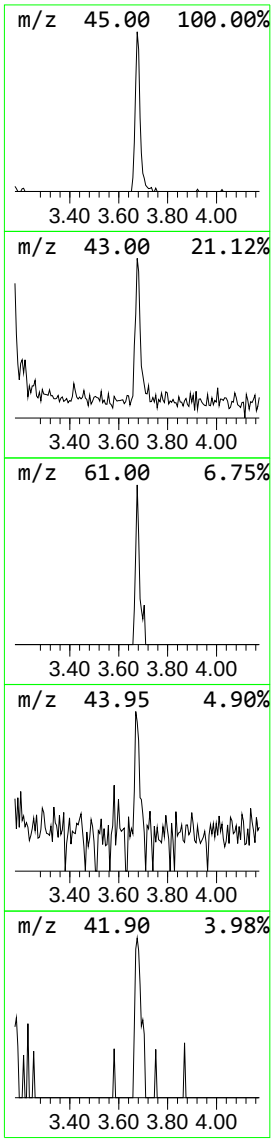
****

Peak Number 2 unknown3.675 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.675	3.39 ng	29809	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Formamide	45	CH3NO	000075-12-7	5
5	L-Lactic acid	90	C3H6O3	000079-33-4	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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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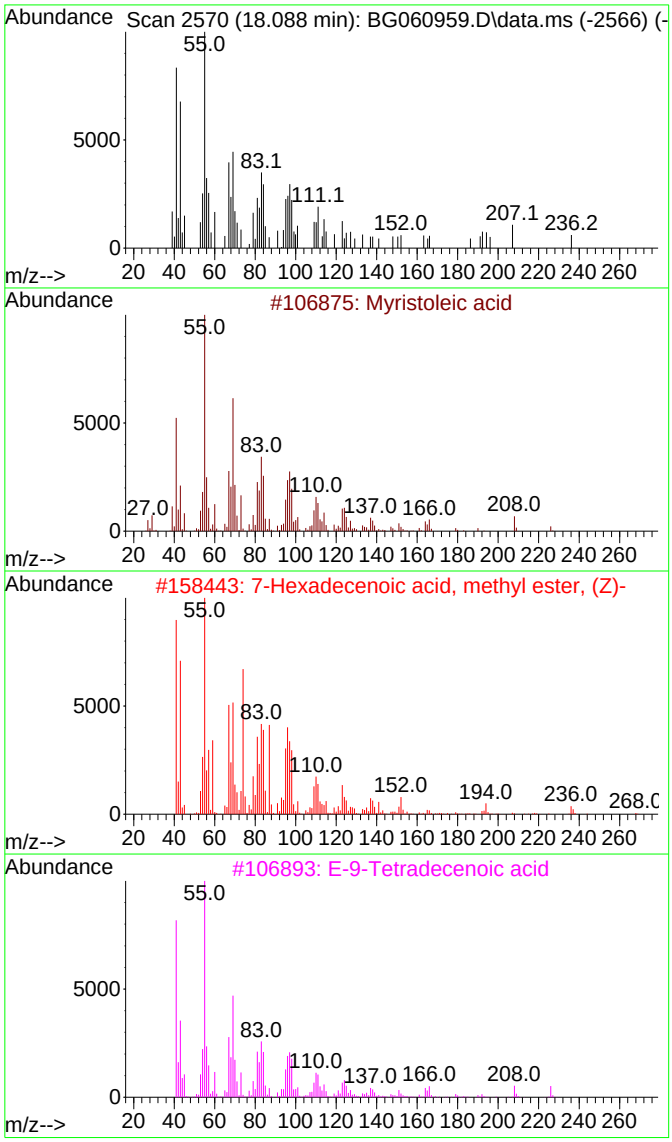
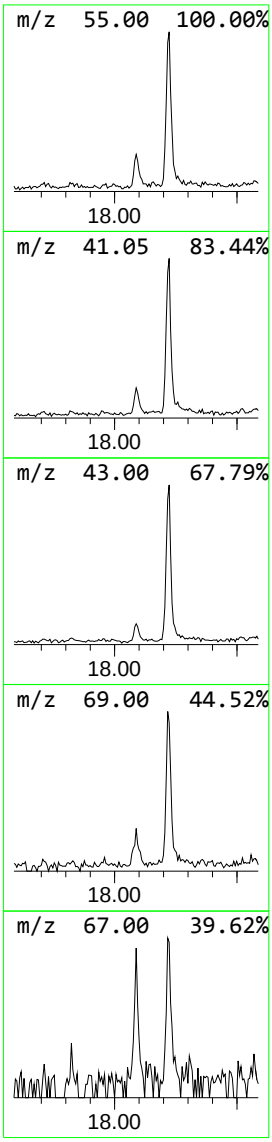
Peak Number 3 Myristoleic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.088	2.23 ng	56847	Phenanthrene-d10	17.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristoleic acid	226	C14H26O2	000544-64-9	80
2	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	72
3	E-9-Tetradecenoic acid	226	C14H26O2	050286-30-1	68
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	68
5	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

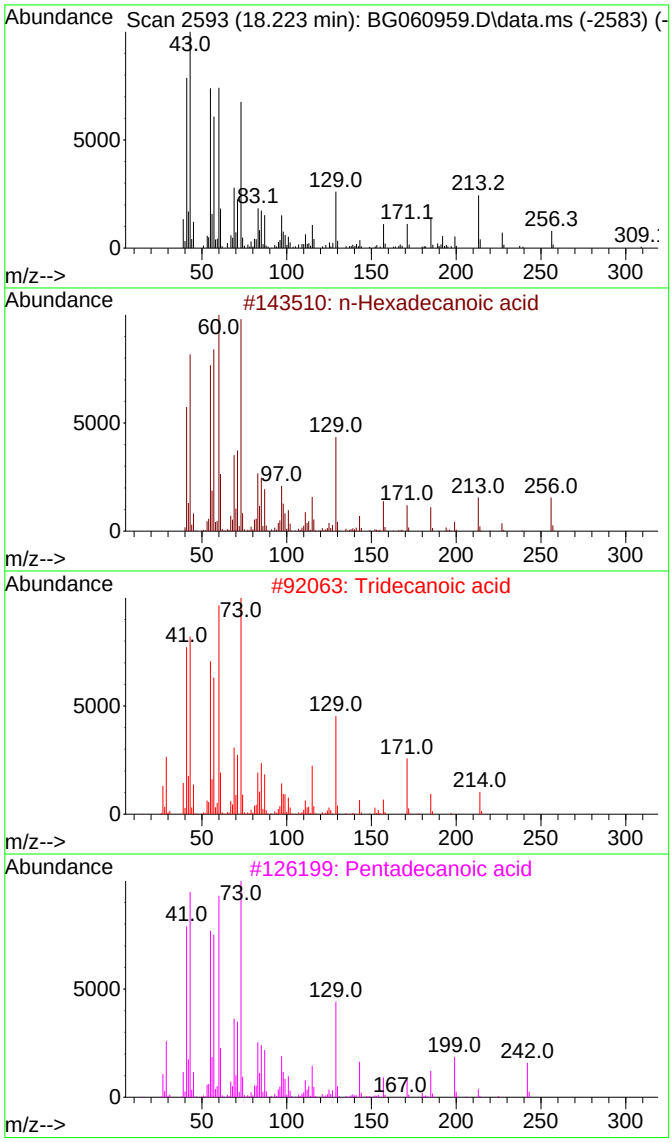
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

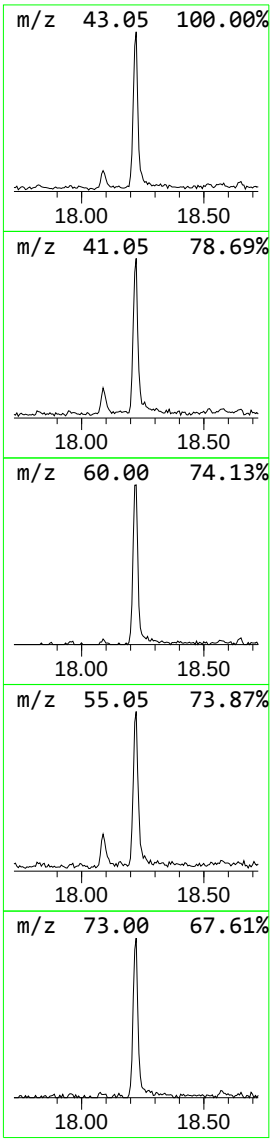
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.223	14.47 ng	368130	Phenanthrene-d10	17.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Octadecanoic acid	284	C18H36O2	000057-11-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

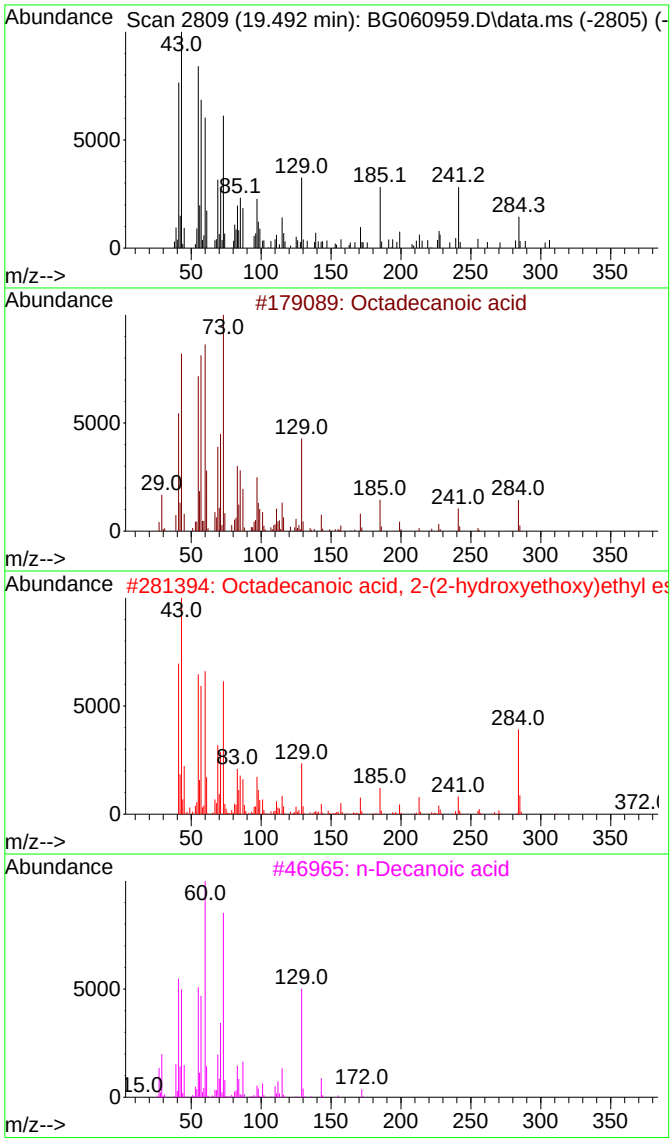
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

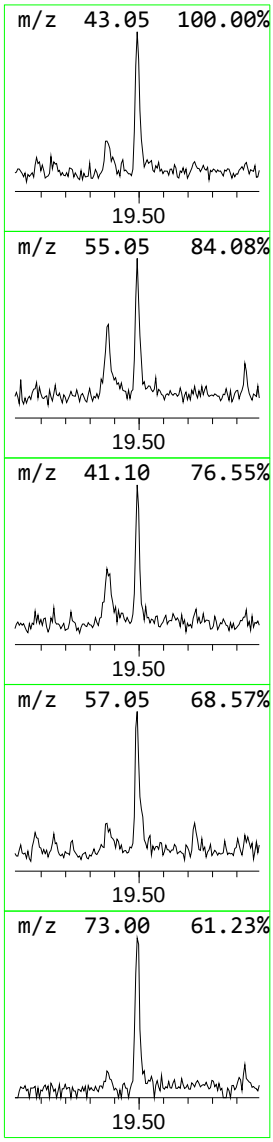
****

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	2.16 ng	86906	Chrysene-d12	21.572

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	92
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	51
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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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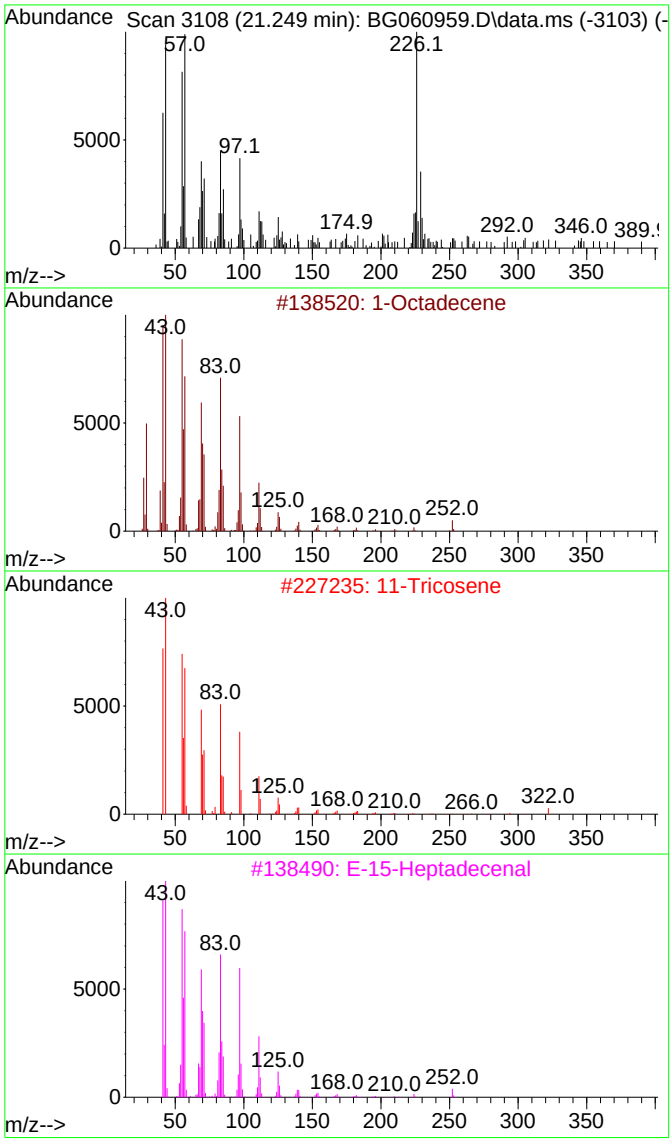
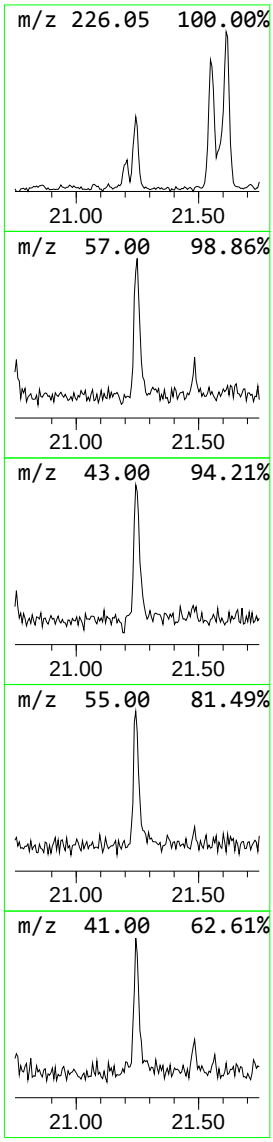
Peak Number 6 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.249	3.31 ng	133372	Chrysene-d12	21.572

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	11-Tricosene	322	C23H46	052078-56-5	93
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	92
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	78
5	1-Heptadecene	238	C17H34	006765-39-5	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

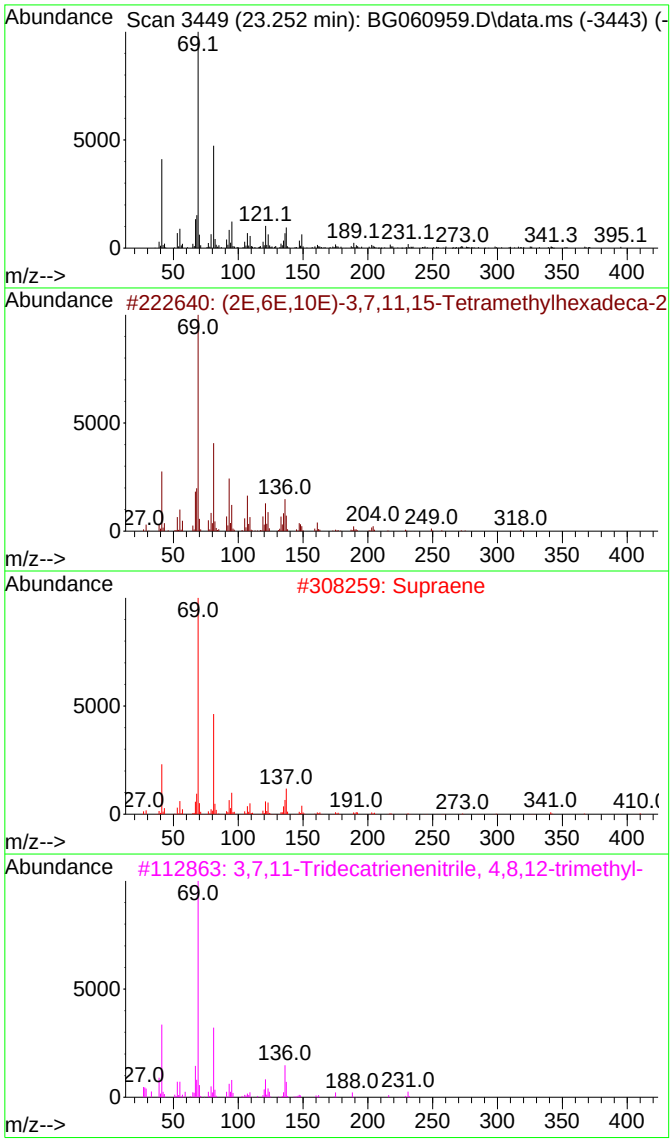
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

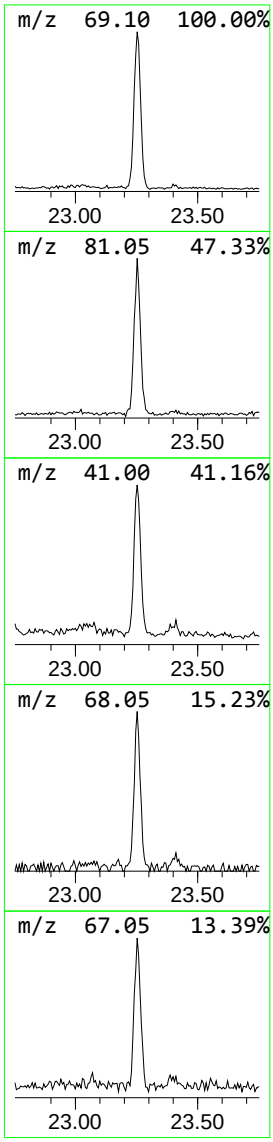
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (2E,6E,10E)-3,7,11,15-Tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.252	11.14 ng	343879	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	83
2	Supraene	410	C30H50	007683-64-9	83
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	80
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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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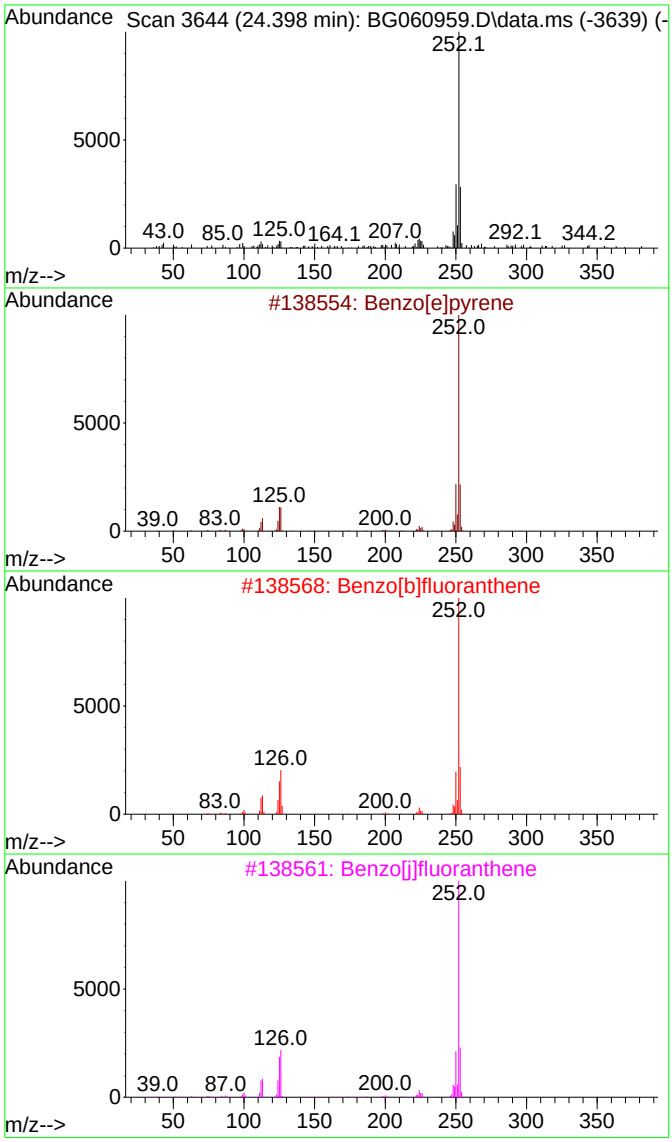
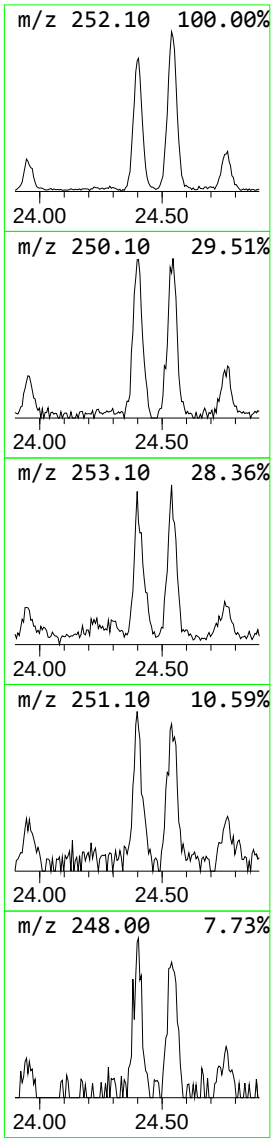
Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.398	4.12 ng	127255	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	81
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5	Benzo[a]pyrene	252	C20H12	000050-32-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041924\
Data File : BG060959.D
Acq On : 19 Apr 2024 14:52
Operator : MA/JU
Sample : P2187-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR200027-E2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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...	3.164	4.5	ng	39848	1	7.941	176099	20.0
unknown3.675	3.675	3.4	ng	29809	1	7.941	176099	20.0
Myristoleic acid	18.088	2.2	ng	56847	4	17.312	508818	20.0
n-Hexadecanoic ...	18.223	14.5	ng	368130	4	17.312	508818	20.0
Octadecanoic acid	19.492	2.2	ng	86906	5	21.572	805703	20.0
1-Octadecene	21.249	3.3	ng	133372	5	21.572	805703	20.0
(2E,6E,10E)-3,7...	23.252	11.1	ng	343879	6	24.692	617523	20.0
Benzo[e]pyrene	24.398	4.1	ng	127255	6	24.692	617523	20.0