LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RT-80-W-ROCKAWAY-B-2

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-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.613	379	387	398	rBV	370076	605106	56.04%	8.496%
2	7.229	654	662	673	rBV	400381	689305	63.84%	9.678%
3	8.063	797	804	810	rBV2	101620	166272	15.40%	2.335%
4	9.238	994	1004	1012	rBV	257154	455222	42.16%	6.392%
5	10.889	1277	1285	1292	rBV	126173	221697	20.53%	3.113%
6	13.339	1695	1702	1710	rVB	564974	875563	81.09%	12.294%
7	14.162	1838	1842	1847	rVB2	13108	17851	1.65%	0.251%
8	14.720	1931	1937	1945	rBV	188243	291993	27.04%	4.100%
9	16.218	2185	2192	2202	rBV	463278	719266	66.61%	10.099%
10	16.453	2228	2232	2236	rVB4	8589	12005	1.11%	0.169%
11	16.547	2243	2248	2253	rBV2	19886	27184	2.52%	0.382%
12	16.606	2253	2258	2263	rVV4	18962	36178	3.35%	0.508%
13	16.665	2263	2268	2271	rVV2	18144	24713	2.29%	0.347%
14	16.706	2271	2275	2281	rVB5	10954	18203	1.69%	0.256%
15	16.864	2297	2302	2309	rVB4	15429	31108	2.88%	0.437%
16	16.935	2309	2314	2318	rVV	19378	29877	2.77%	0.419%
17	17.011	2322	2327	2332	rVB3	9757	16519	1.53%	0.232%
18	17.481	2401	2407	2412	rBV	231285	353386	32.73%	4.962%
19	17.746	2448	2452	2456	rBV	9082	14383	1.33%	0.202%
20	18.363	2552	2557	2562	rBV4	11461	26994	2.50%	0.379%
21	18.433	2565	2569	2574	rVB2	11889	20336	1.88%	0.286%
22	18.856	2638	2641	2647	rVB4	7339	12489	1.16%	0.175%
23	18.956	2654	2658	2663	rBV5	6141	12656	1.17%	0.178%
24	19.121	2676	2686	2690	rBV	44137	69627	6.45%	0.978%
25	19.209	2697	2701	2706	rBV6	9775	17211	1.59%	0.242%
26	19.273	2708	2712	2716	rBV7	8859	15657	1.45%	0.220%
27	19.538	2751	2757	2761	rBV3	34038	55474	5.14%	0.779%
28	19.755	2790	2794	2797	rVV3	10254	13242	1.23%	0.186%
29	19.902	2815	2819	2826	rVB	51232	66881	6.19%	0.939%
30	20.090	2846	2851	2857	rBV	823223	1079784	100.00%	15.161%
31	20.355	2893	2896	2899	rBV5	8239	11993	1.11%	0.168%
32	20.384	2899	2901	2905	rVB5	8794	11137	1.03%	0.156%
33	20.766	2963	2966	2970	rVB	28601	36865	3.41%	0.518%
34	20.848	2973	2980	2983	rBV8	11992	24447	2.26%	0.343%
35	20.983	2998	3003	3007	rBV	82919	108827	10.08%	1.528%
36	21.030	3008	3011	3015	rVB4	17305	22611	2.09%	0.317%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RT-80-W-ROCKAWAY-B-2

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-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.394	3068	3073	3080	rBV2	74259	98682	9.14%	1.386%
38	21.647	3113	3116	3119	rVB4	9180	11900	1.10%	0.167%
39	21.782	3132	3139	3146	rBV	196913	341633	31.64%	4.797%
40	21.970	3167	3171	3175	rBV7	7375	10974	1.02%	0.154%
41	22.587	3270	3276	3278	rBV7	18862	35093	3.25%	0.493%
42	24.050	3521	3525	3527	rBV5	10947	16088	1.49%	0.226%
43	24.127	3535	3538	3546	rVB10	20402	46483	4.30%	0.653%
44	25.114	3698	3706	3717	rVB2	119804	332817	30.82%	4.673%
45	28.545	4284	4290	4292	rBV7	7700	16382	1.52%	0.230%

Sum of corrected areas: 7122114

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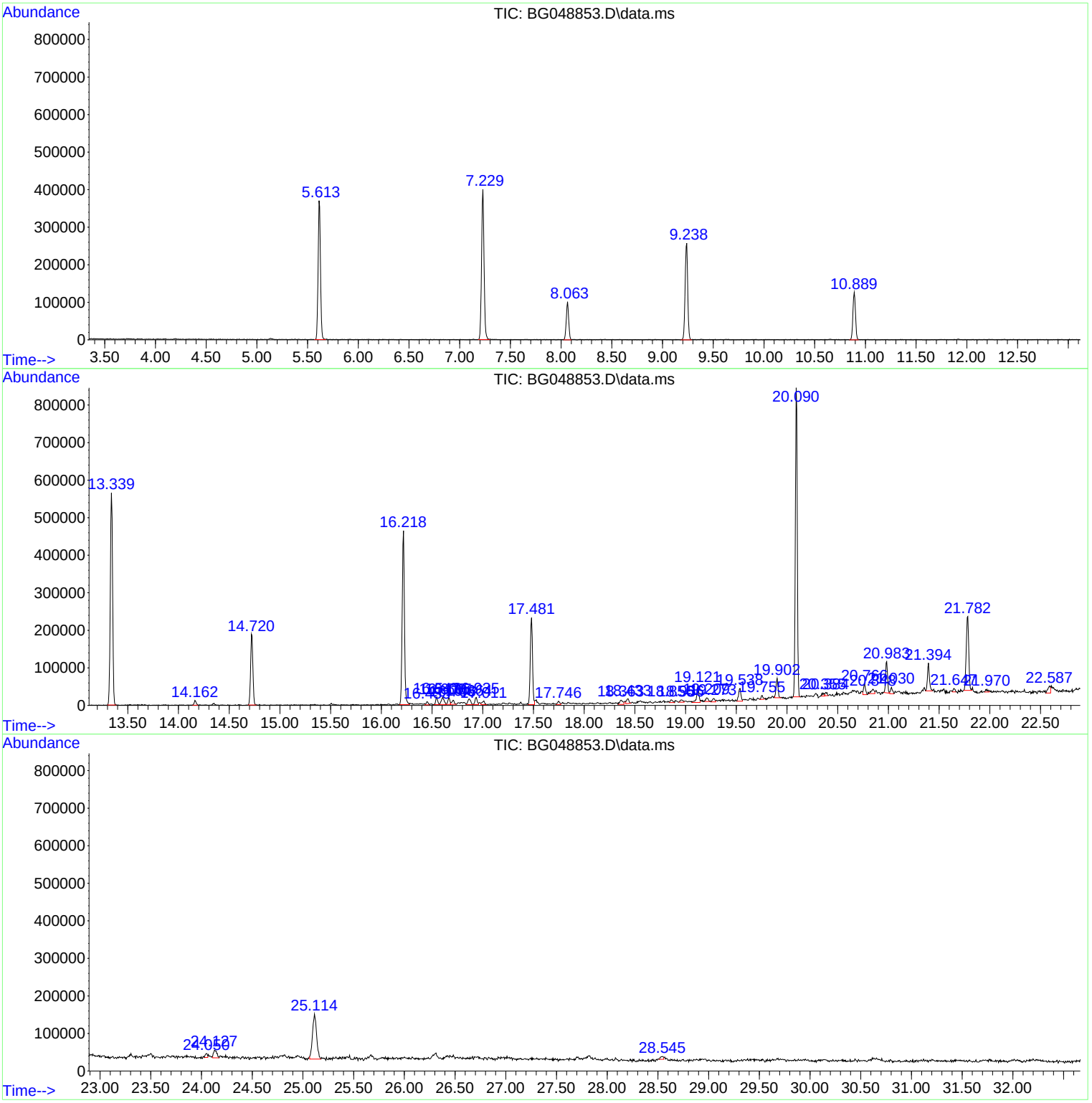
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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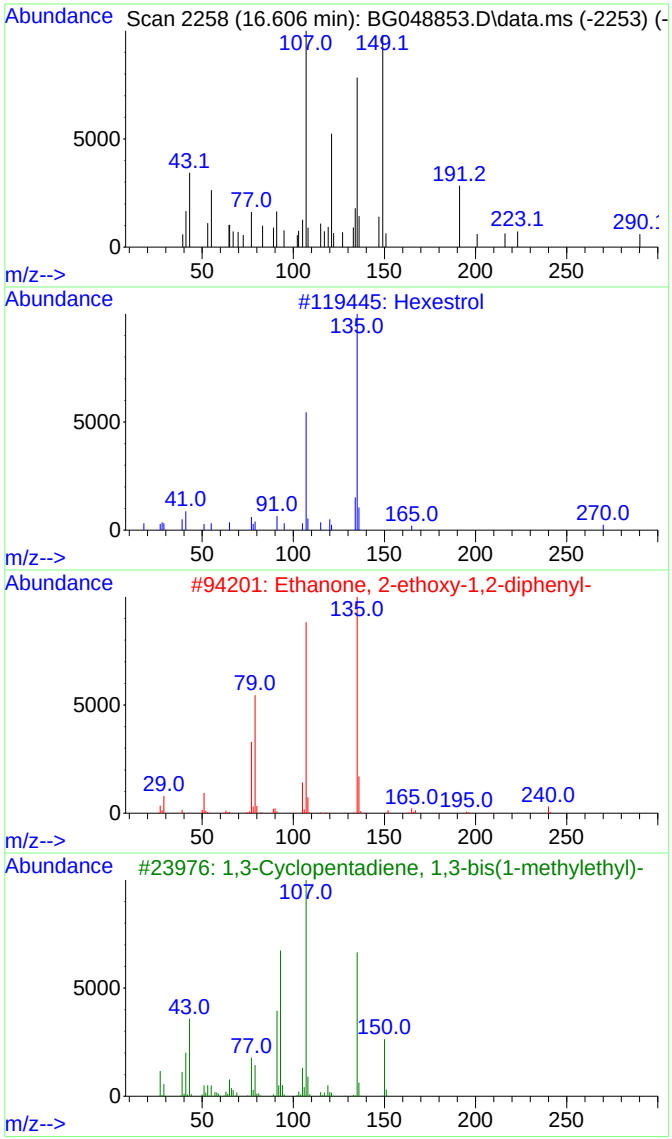
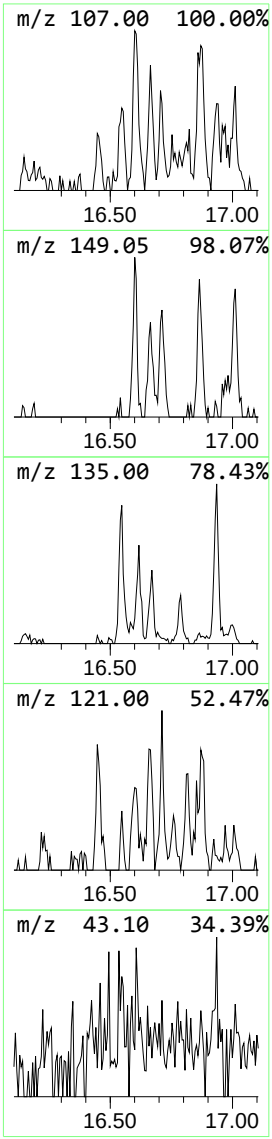
Peak Number 1 unknown16.606 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.606	2.05 ng	36178	Phenanthrene-d10	17.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexestrol	270	C18H22O2	005635-50-7	43
2	Ethanone, 2-ethoxy-1,2-diphenyl-	240	C16H16O2	000574-09-4	43
3	1,3-Cyclopentadiene, 1,3-bis(1-m...	150	C11H18	123278-27-3	43
4	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	43
5	Benzene, (1-ethoxy-3-butenyl)-	176	C12H16O	054703-48-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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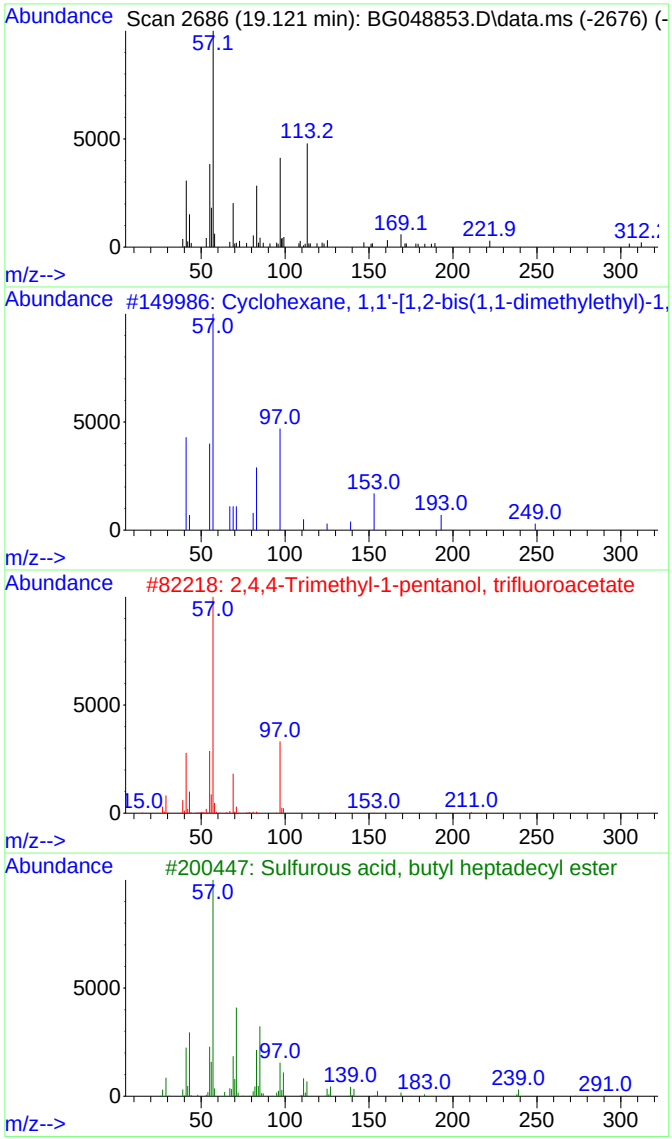
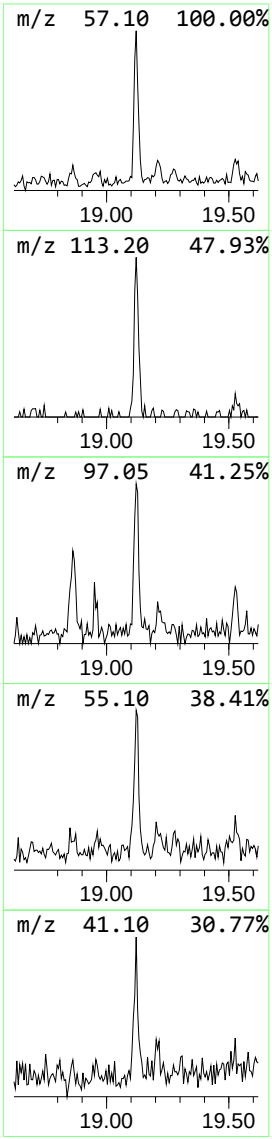
Peak Number 2 unknown19.121 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.121	3.94 ng	69627	Phenanthrene-d10	17.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	37
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	16
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	14
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RT-80-W-ROCKAWAY-B-2

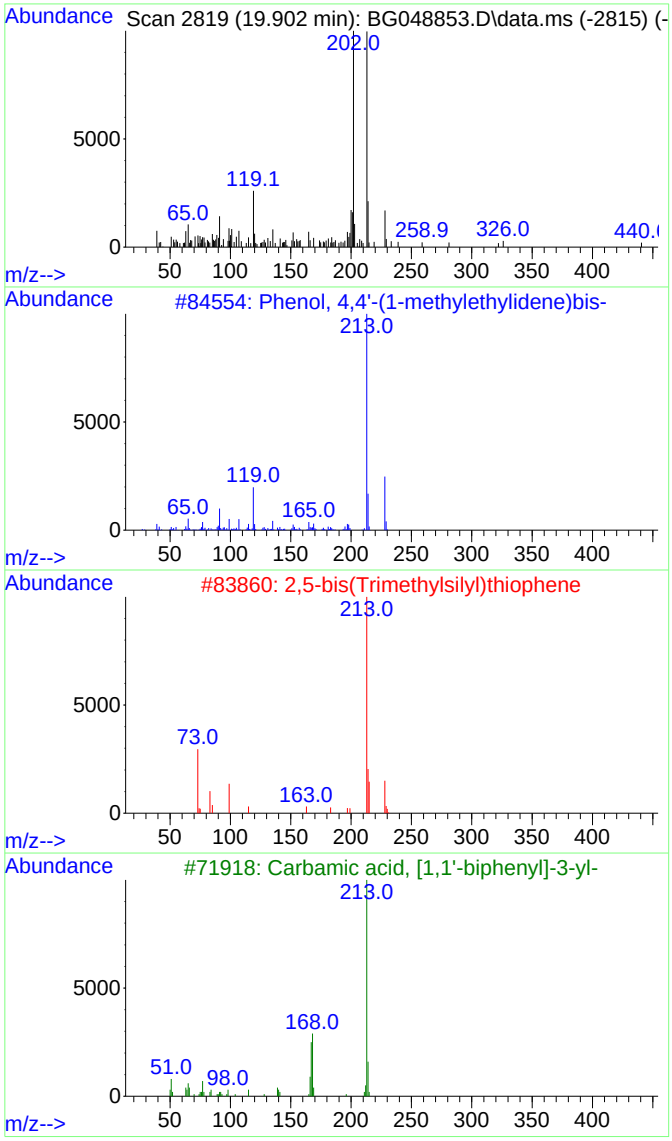
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

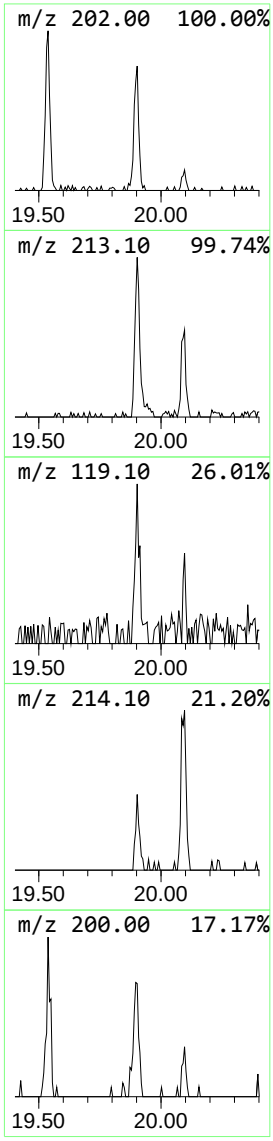
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.902	3.92 ng	66881	Chrysene-d12	21.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	35
3	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	30
4	4H-Pyrrolo[2,3-c]pyrazole-1-carb...	366	C20H19ClN4O	1000296-35-2	27
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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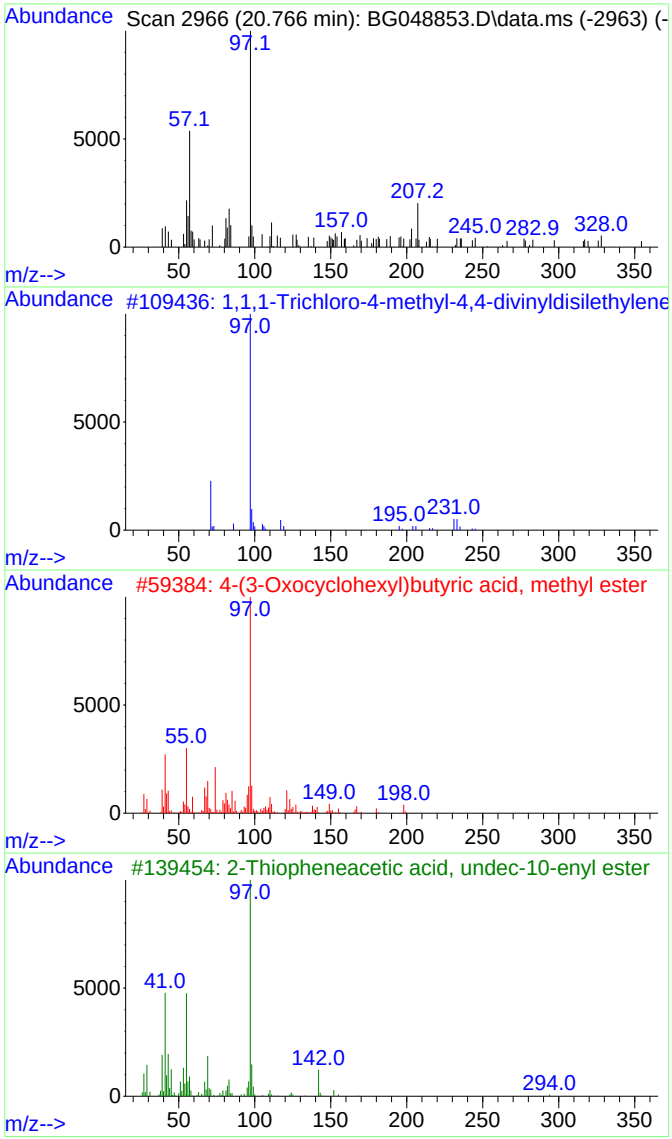
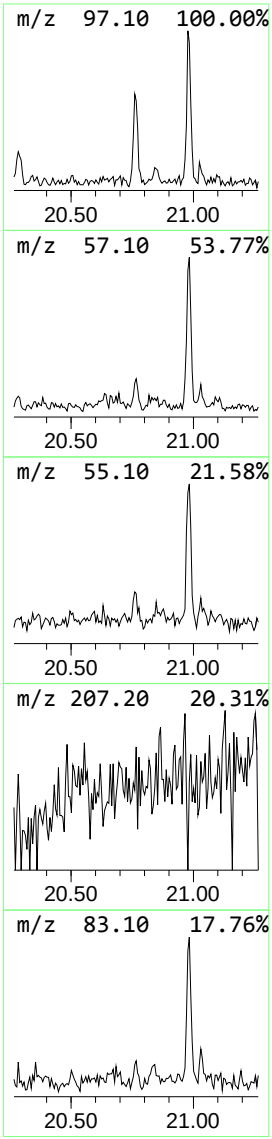
Peak Number 5 unknown20.766 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.766	2.16 ng	36865	Chrysene-d12	21.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1-Trichloro-4-methyl-4,4-div...	258	C7H13Cl3Si2	102105-46-4	47
2	4-(3-Oxocyclohexyl)butyric acid,...	198	C11H18O3	147895-12-3	46
3	2-Thiopheneacetic acid, undec-10...	294	C17H26O2S	1000278-91-6	43
4	Cyclohexane, 1,5-diisopropyl-2,3...	196	C14H28	1000149-58-8	43
5	Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
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Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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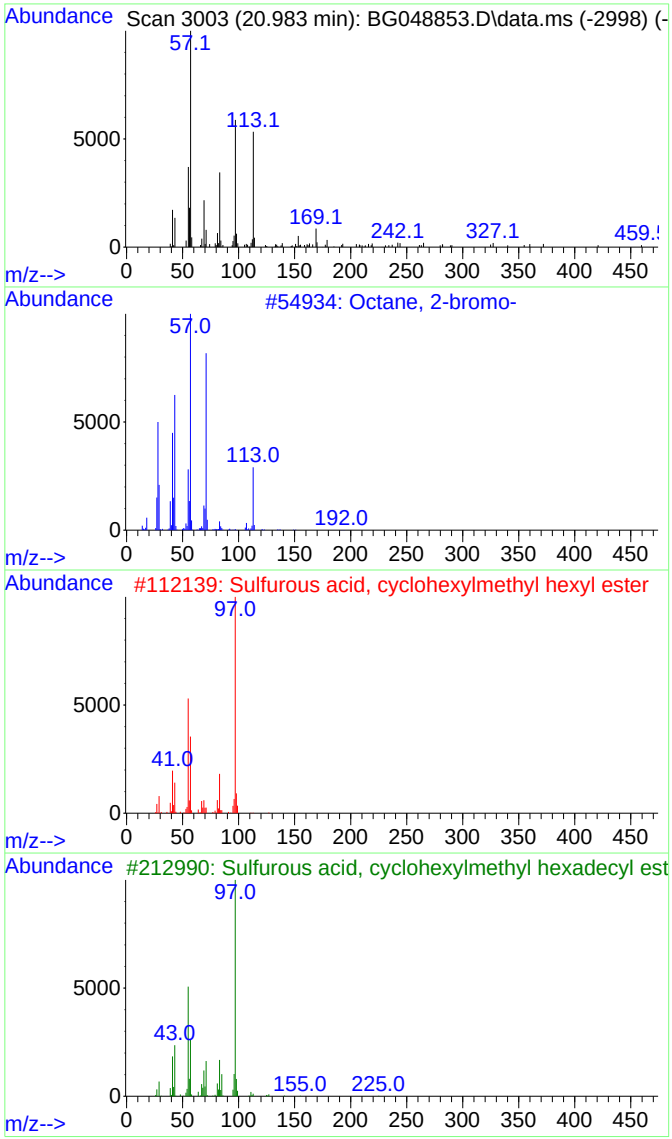
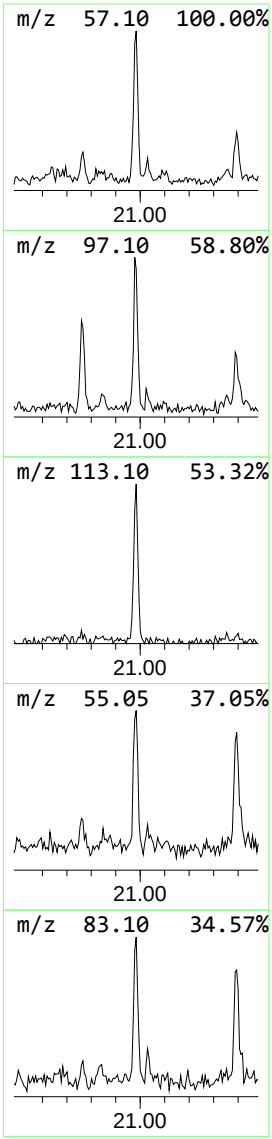
Peak Number 6 unknown20.983 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.983	6.37 ng	108827	Chrysene-d12	21.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
2	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	27
3	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	27
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	27
5	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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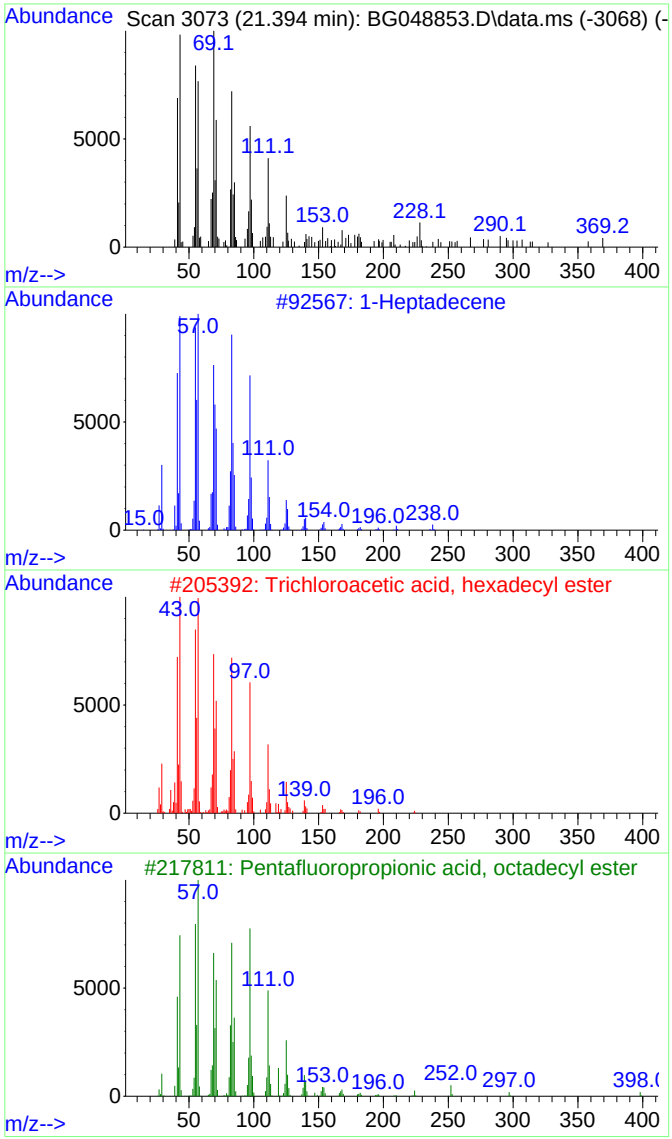
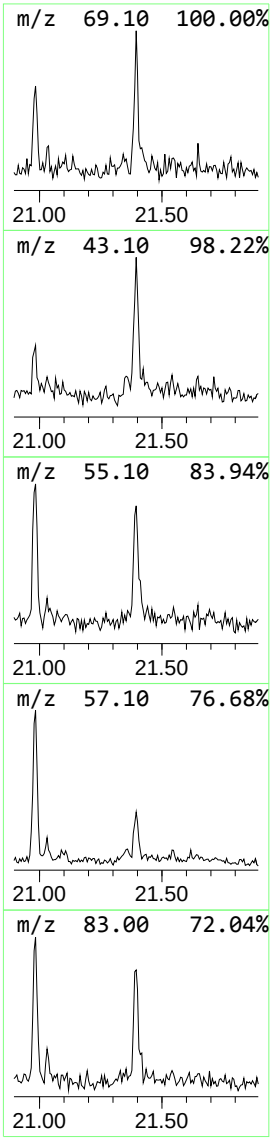
Peak Number 7 1-Heptadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.395	5.78 ng	98682	Chrysene-d12	21.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	86
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	70
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	70
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	70





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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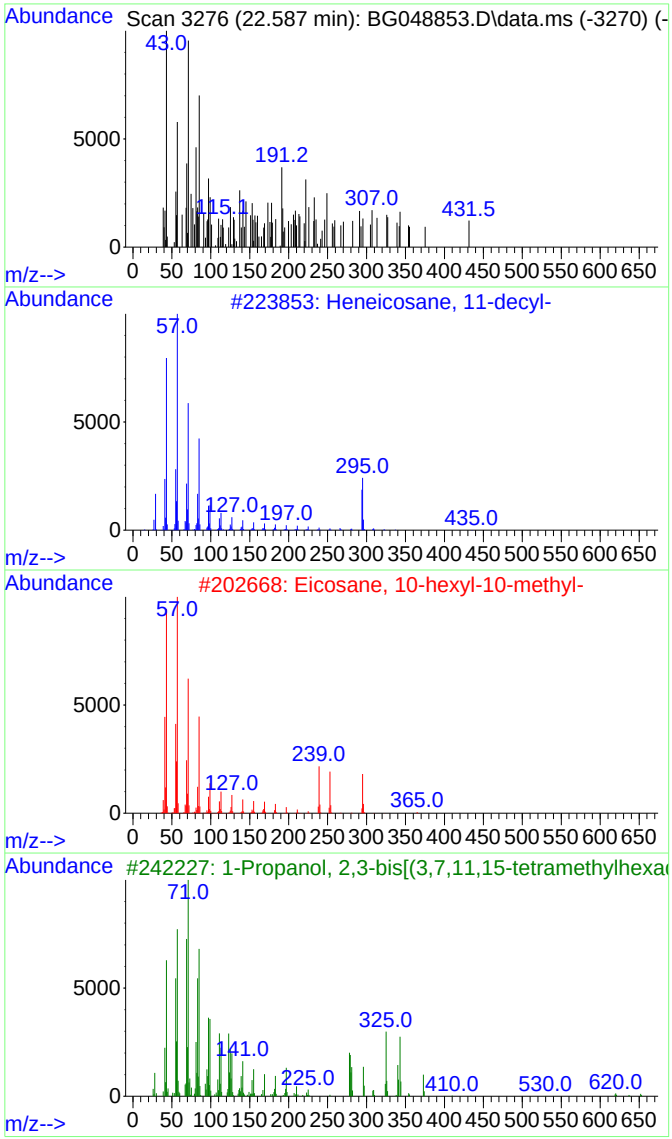
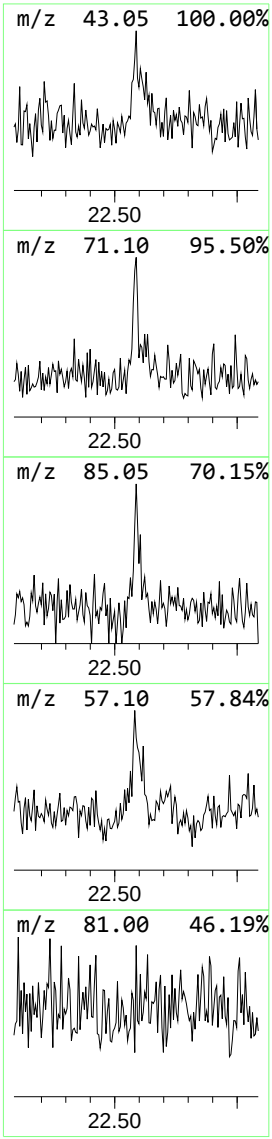
Peak Number 8 unknown22.587 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.587	2.05 ng	35093	Chrysene-d12	21.782

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	32
2	Eicosane, 10-hexyl-10-methyl-	380	C27H56	055282-32-1	32
3	1-Propanol, 2,3-bis[(3,7,11,15-t...	653	C43H88O3	006540-63-2	25
4	13,17,21-Trimethylheptatriacontane	563	C40H82	058668-40-9	23
5	Eicosane	282	C20H42	000112-95-8	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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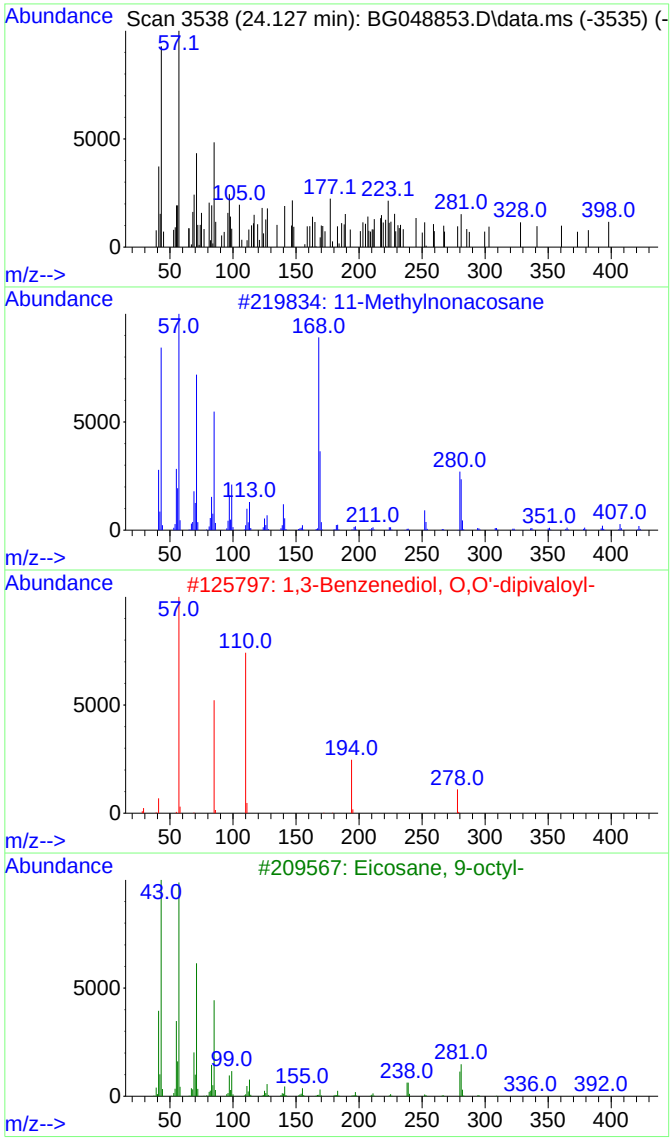
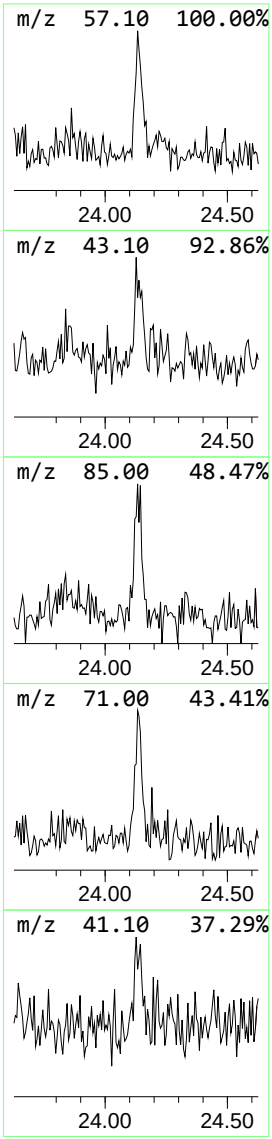
Peak Number 9 unknown24.127 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.127	2.79 ng	46483	Perylene-d12	25.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Methylnonacosane	422	C30H62	007371-99-5	17
2	1,3-Benzenediol, O,O'-dipivaloyl-	278	C16H22O4	1000330-67-7	12
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	12
4	Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	12
5	1-Bromoeicosane	360	C20H41Br	004276-49-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048853.D
Acq On : 22 Apr 2021 19:04
Operator : CG/JU
Sample : M2036-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RT-80-W-ROCKAWAY-B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown16.606	16.606	2.0	ng	36178	4	17.481	353386	20.0
unknown19.121	19.121	3.9	ng	69627	4	17.481	353386	20.0
Phenol, 4,4'-(1...	19.902	3.9	ng	66881	5	21.782	341633	20.0
unknown20.766	20.766	2.2	ng	36865	5	21.782	341633	20.0
unknown20.983	20.983	6.4	ng	108827	5	21.782	341633	20.0
1-Heptadecene	21.395	5.8	ng	98682	5	21.782	341633	20.0
unknown22.587	22.587	2.0	ng	35093	5	21.782	341633	20.0
unknown24.127	24.127	2.8	ng	46483	6	25.114	332817	20.0