LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CONC-COMP

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.306	202	207	222	rVB	267616	377113	21.39%	2.780%
2	4.911	303	310	318	rBV	314916	470044	26.66%	3.465%
3	5.381	384	390	405	rBV	363916	576569	32.70%	4.250%
4	6.979	655	662	675	rBV	410648	713399	40.46%	5.259%
5	7.808	796	803	810	rBV	131232	216593	12.28%	1.597%
6	8.971	994	1001	1018	rBV	263252	489701	27.77%	3.610%
7	10.610	1272	1280	1287	rBV	177784	332425	18.85%	2.450%
8	13.078	1693	1700	1712	rBV	755565	1185096	67.21%	8.736%
9	13.343	1739	1745	1758	rVB	267798	433745	24.60%	3.197%
10	14.453	1928	1934	1941	rBV	299147	485166	27.51%	3.576%
11	14.518	1941	1945	1955	rVB	31356	49137	2.79%	0.362%
12	14.858	1997	2003	2011	rBV	27901	44828	2.54%	0.330%
13	15.505	2108	2113	2124	rBV	62990	99664	5.65%	0.735%
14	15.798	2159	2163	2170	rVB	13018	18923	1.07%	0.139%
15	15.945	2183	2188	2199	rBV	327461	561721	31.86%	4.141%
16	16.509	2277	2284	2289	rVB4	11709	23065	1.31%	0.170%
17	17.021	2366	2371	2381	rVB	18197	27227	1.54%	0.201%
18	17.203	2395	2402	2406	rBV	412561	623124	35.34%	4.593%
19	17.244	2406	2409	2417	rVV	359082	501659	28.45%	3.698%
20	17.338	2417	2425	2430	rVV	102896	165776	9.40%	1.222%
21	17.402	2430	2436	2440	rVB3	9418	18032	1.02%	0.133%
22	17.614	2462	2472	2481	rBV2	39521	78548	4.45%	0.579%
23	18.078	2544	2551	2555	rBV	35255	58218	3.30%	0.429%
24	18.125	2555	2559	2568	rVB	54646	86602	4.91%	0.638%
25	18.207	2568	2573	2578	rBV	21445	31821	1.80%	0.235%
26	18.278	2578	2585	2589	rVV3	54852	100085	5.68%	0.738%
27	18.307	2589	2590	2596	rVB	21081	23565	1.34%	0.174%
28	18.578	2631	2636	2641	rBV	21562	29360	1.67%	0.216%
29	19.001	2702	2708	2711	rBV4	21248	38727	2.20%	0.285%
30	19.036	2711	2714	2718	rVV3	39139	46199	2.62%	0.341%
31	19.259	2746	2752	2758	rBV	310425	430265	24.40%	3.172%
32	19.588	2804	2808	2810	rBV	58122	79306	4.50%	0.585%
33	19.623	2810	2814	2822	rVV	206065	313335	17.77%	2.310%
34	19.694	2822	2826	2833	rVB	16008	24266	1.38%	0.179%
35	19.823	2840	2848	2853	rBV	1361231	1763310	100.00%	12.998%
36	19.864	2853	2855	2863	rVB3	17442	27479	1.56%	0.203%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.941	2863	2868	2876	rBV6	17785	54105	3.07%	0.399%
38	20.076	2886	2891	2894	rBV4	15563	29015	1.65%	0.214%
39	20.117	2894	2898	2903	rVB2	79478	107161	6.08%	0.790%
40	20.217	2910	2915	2919	rBV	55016	69992	3.97%	0.516%
41	20.276	2919	2925	2929	rVB3	22010	40982	2.32%	0.302%
42	20.411	2943	2948	2953	rBV2	11345	22550	1.28%	0.166%
43	20.610	2979	2982	2986	rBV	22000	25638	1.45%	0.189%
44	20.869	3023	3026	3032	rVB2	12076	18948	1.07%	0.140%
45	21.045	3051	3056	3059	rBV	19357	26811	1.52%	0.198%
46	21.092	3059	3064	3068	rVV2	46869	83019	4.71%	0.612%
47	21.133	3068	3071	3076	rVB4	19332	35643	2.02%	0.263%
48	21.445	3111	3124	3129	rBV2	433033	907453	51.46%	6.689%
49	21.486	3129	3131	3137	rVB	93558	131925	7.48%	0.972%
50	21.621	3149	3154	3162	rVB4	21575	42182	2.39%	0.311%
51	21.780	3177	3181	3185	rVB2	11424	18225	1.03%	0.134%
52	21.844	3185	3192	3198	rVB3	17596	37671	2.14%	0.278%
53	22.144	3236	3243	3247	rBV2	22762	45110	2.56%	0.333%
54	22.191	3247	3251	3260	rVB5	20185	47139	2.67%	0.347%
55	22.449	3291	3295	3301	rVV5	11910	23341	1.32%	0.172%
56	22.538	3305	3310	3317	rVB5	8722	18923	1.07%	0.139%
57	22.843	3359	3362	3375	rVB8	17627	39886	2.26%	0.294%
58	23.025	3387	3393	3399	rVB2	17362	31318	1.78%	0.231%
59	23.542	3473	3481	3488	rBV2	57133	181590	10.30%	1.339%
60	23.783	3517	3522	3529	rVB3	14964	33132	1.88%	0.244%
61	24.230	3590	3598	3603	rBV3	27889	70307	3.99%	0.518%
62	24.371	3613	3622	3633	rBV4	45099	129060	7.32%	0.951%
63	24.518	3636	3647	3664	rBV	229491	708453	40.18%	5.222%
64	28.014	4230	4242	4243	rBV3	14432	42702	2.42%	0.315%

Sum of corrected areas: 13566374

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
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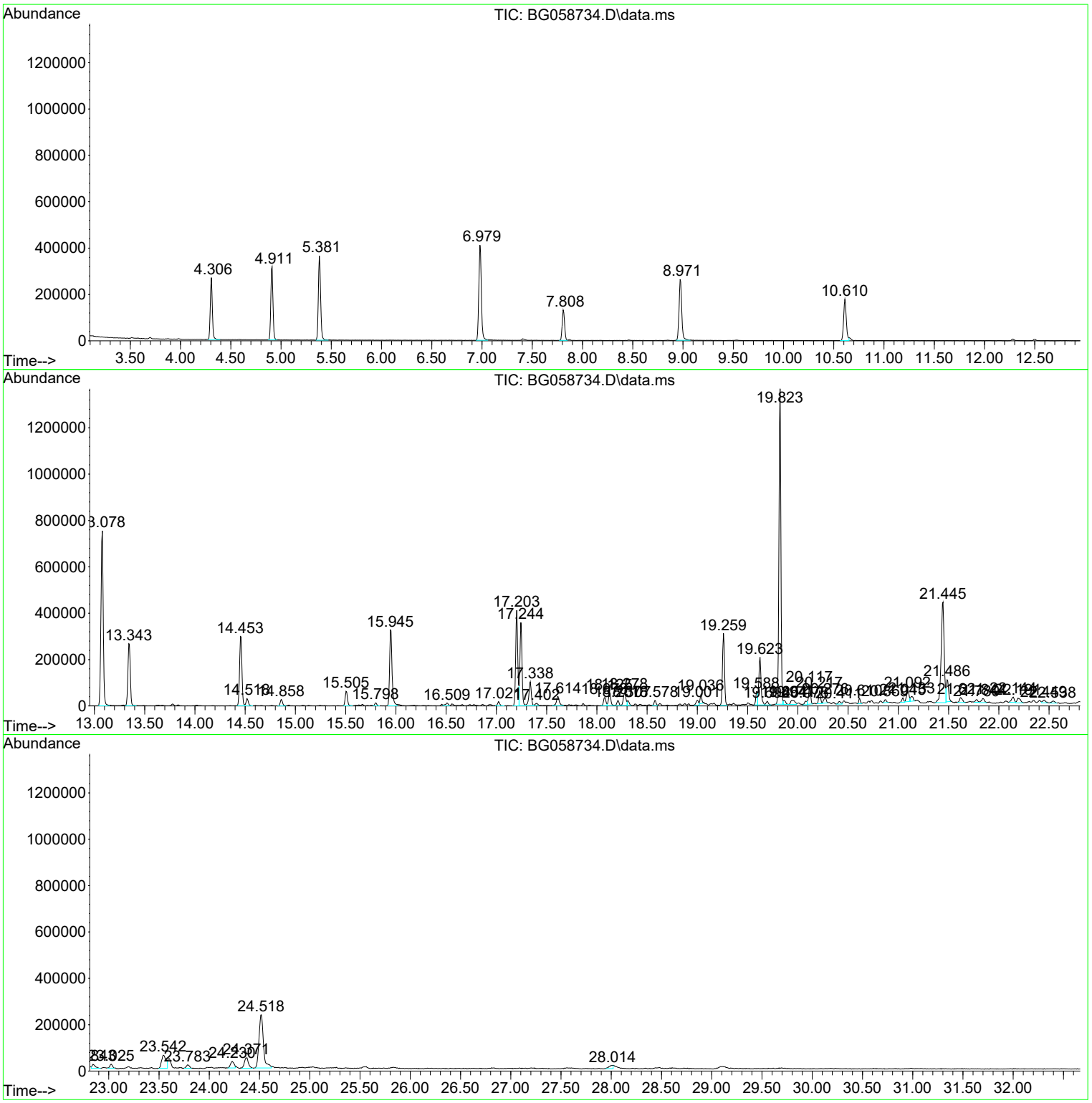
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

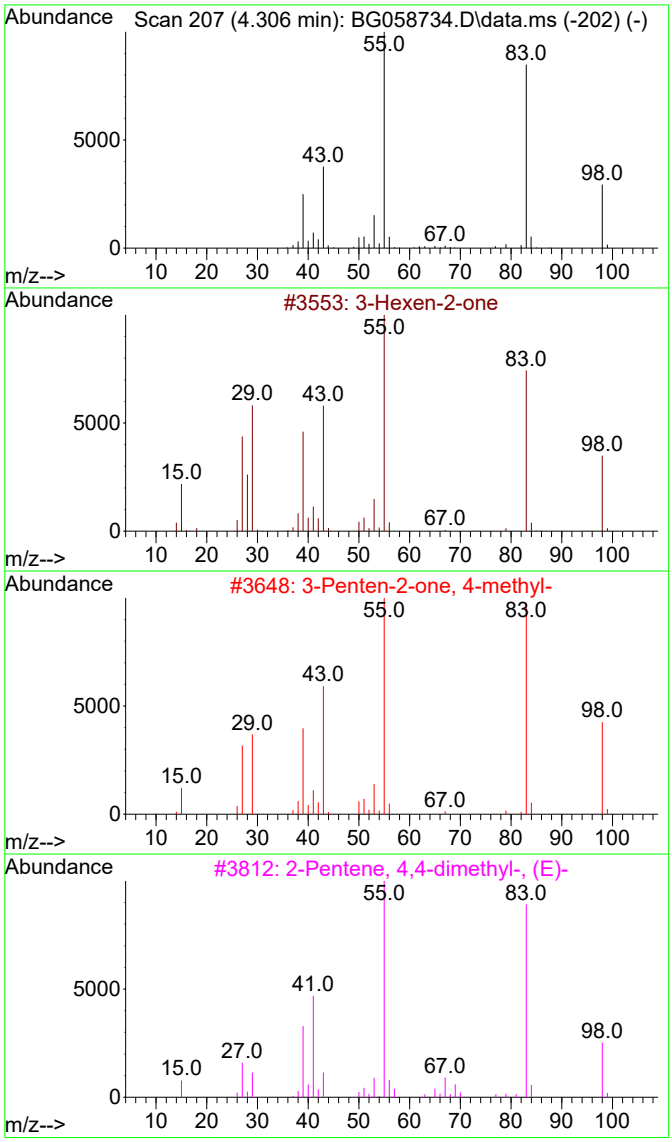
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

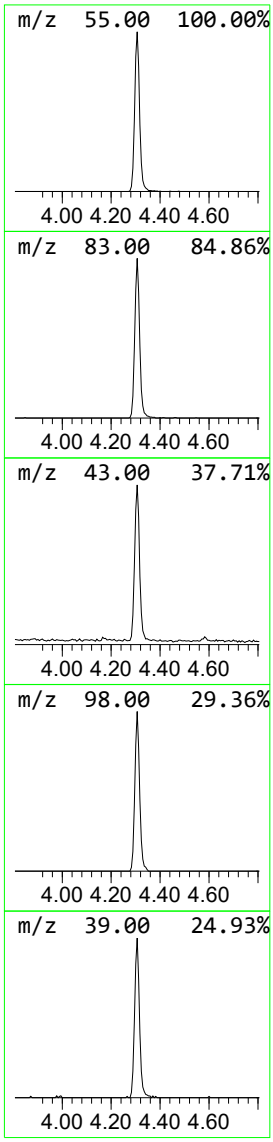
****

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	34.82 ng	377113	1,4-Dichlorobenzene-d4	7.808

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

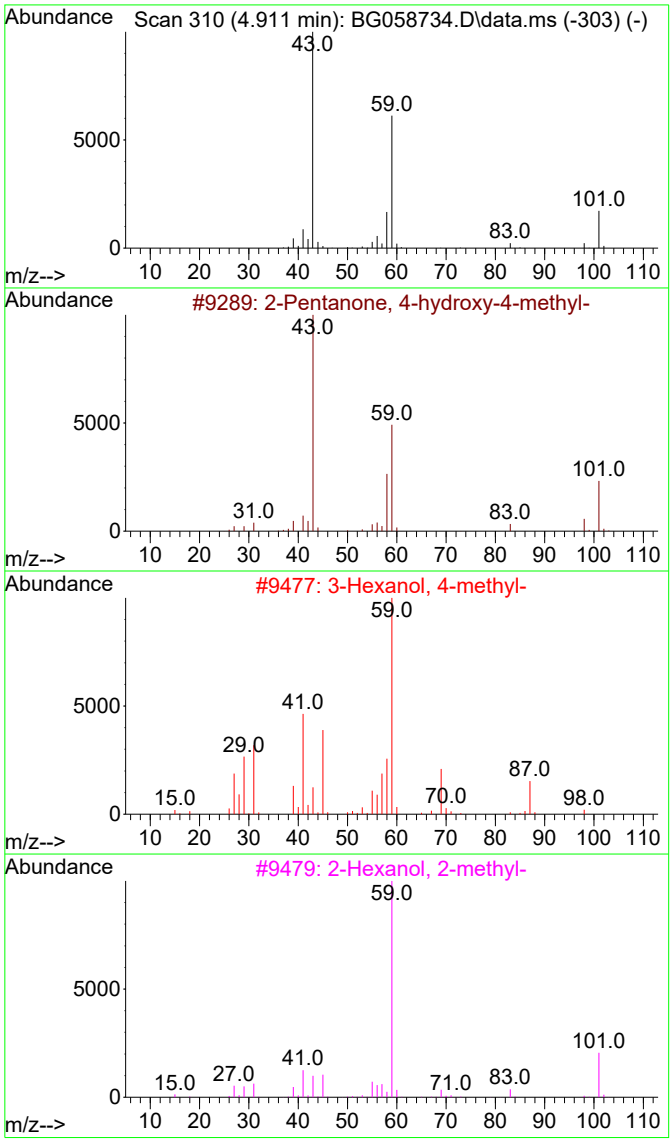
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

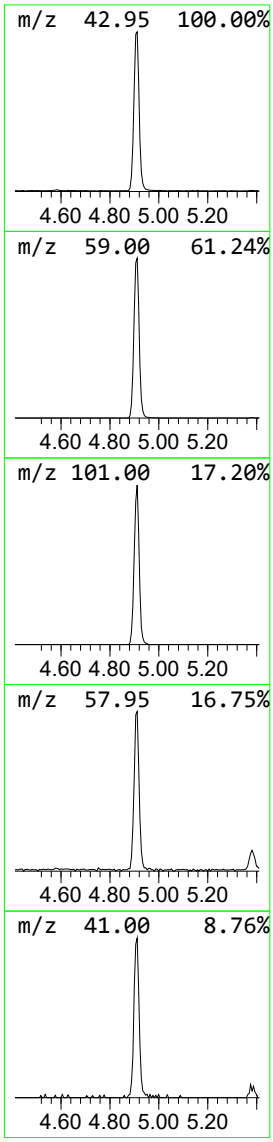
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.911	43.40 ng	470044	1,4-Dichlorobenzene-d4	7.808

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
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	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

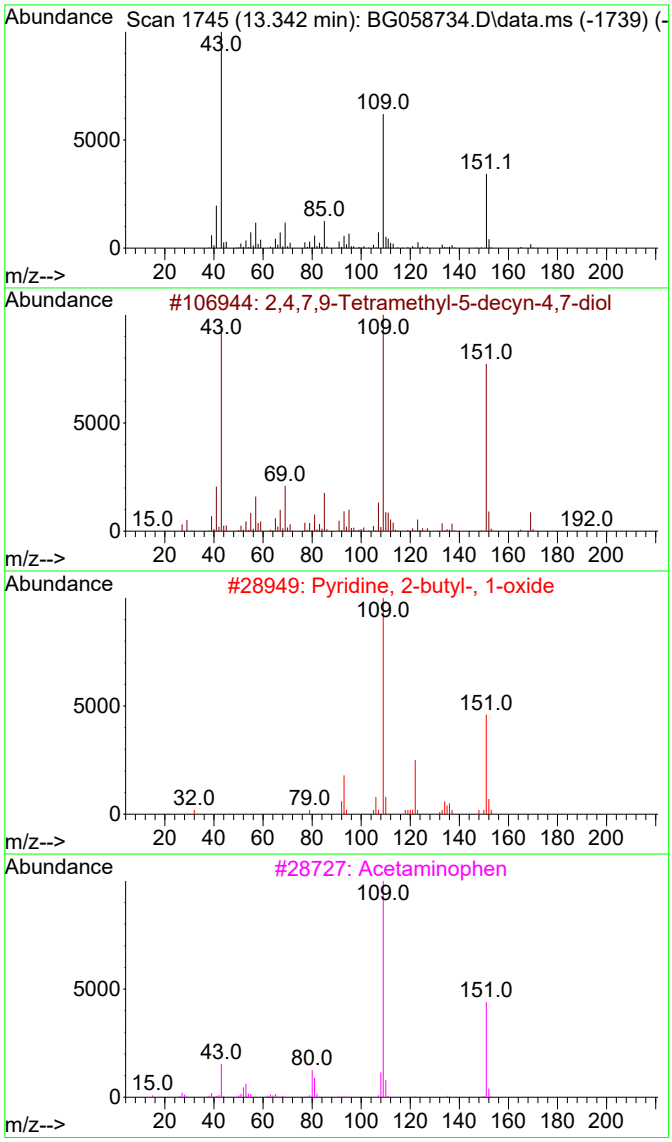
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

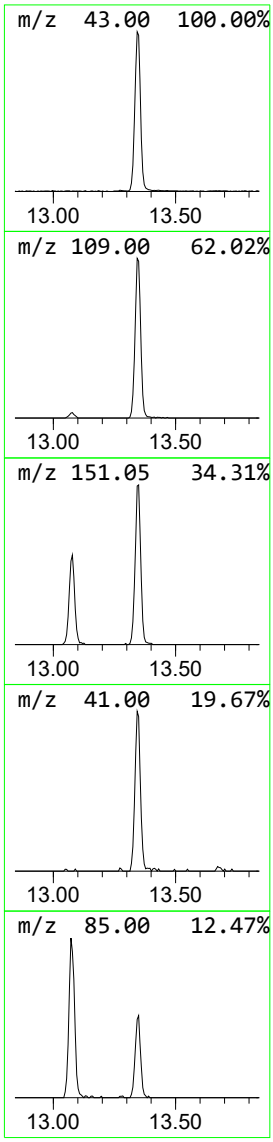
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.342	17.88 ng	433745	Acenaphthene-d10	14.453

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	49
4	Metacetamol	151	C8H9NO2	000621-42-1	47
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

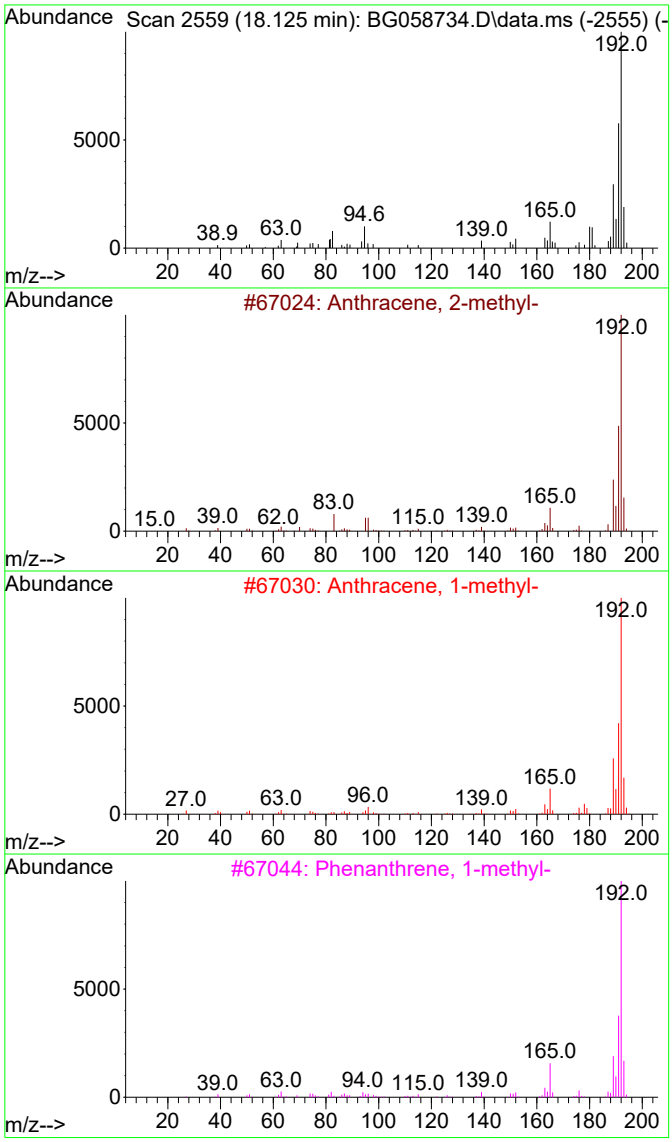
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

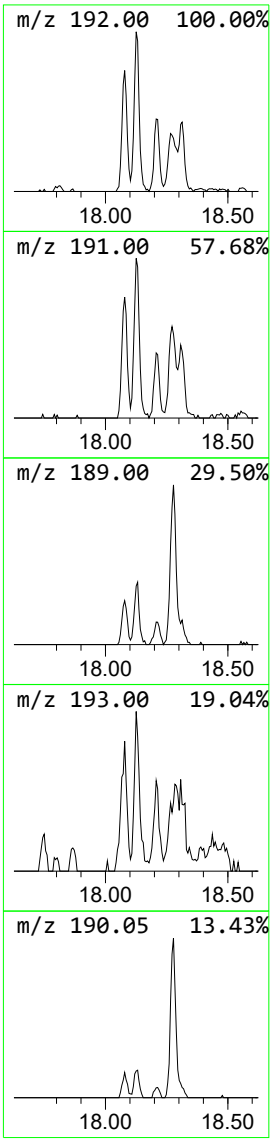
****

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.125	2.78 ng	86602	Phenanthrene-d10	17.203

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	92
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

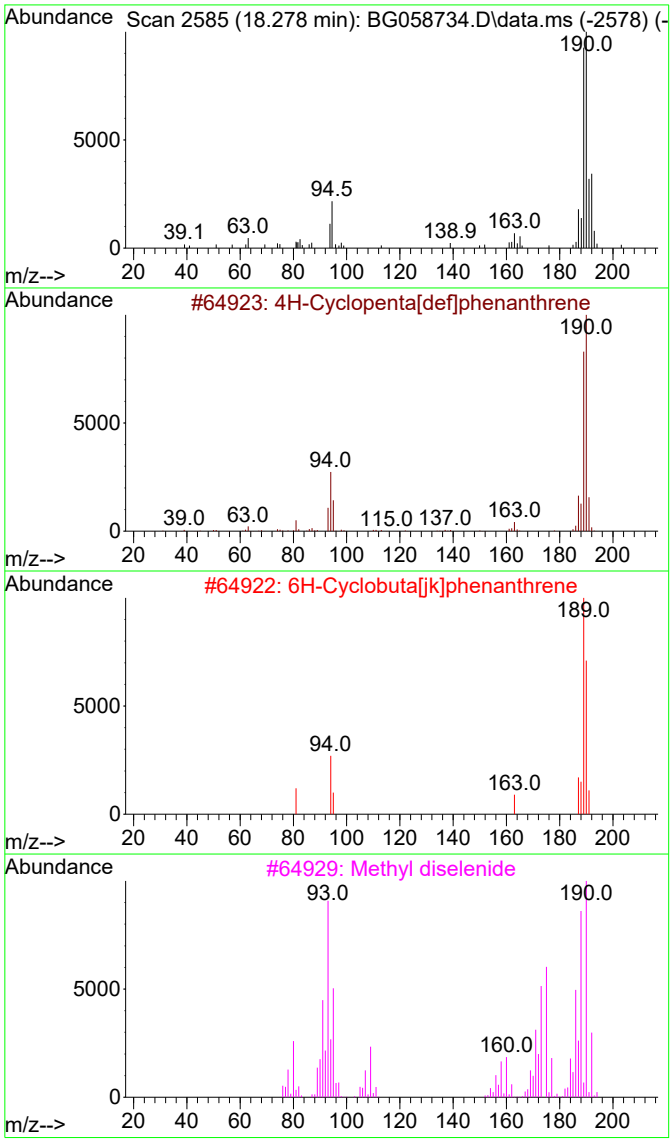
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

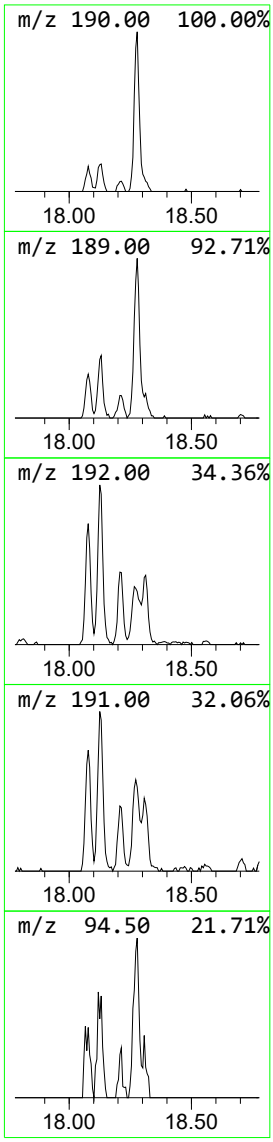
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.278	3.21 ng	100085	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

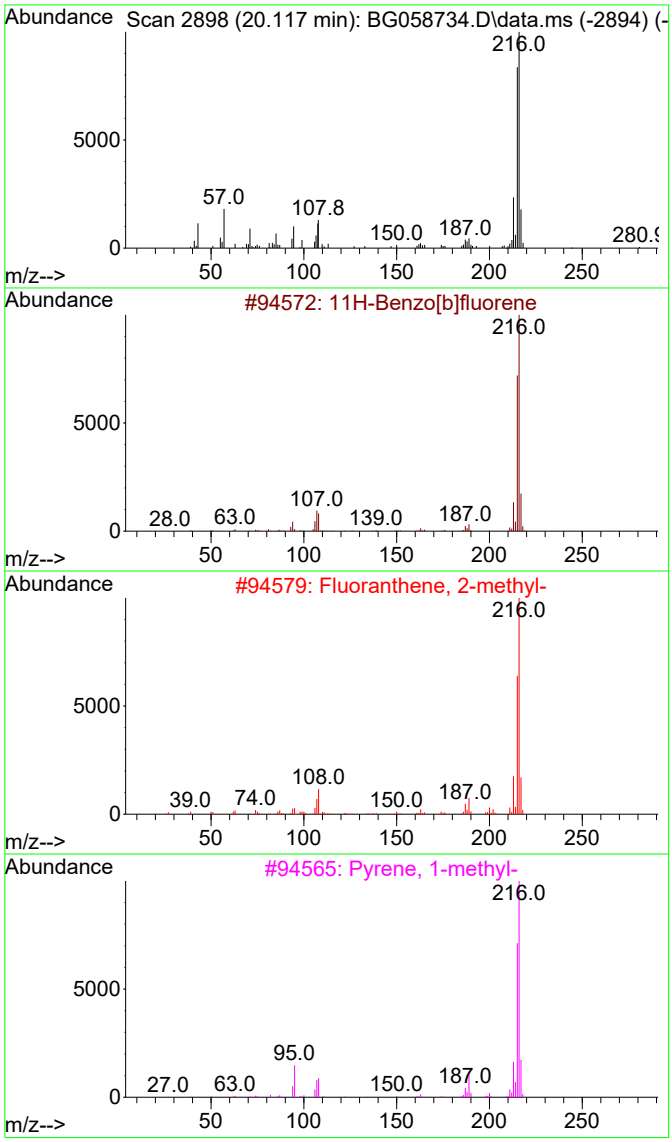
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

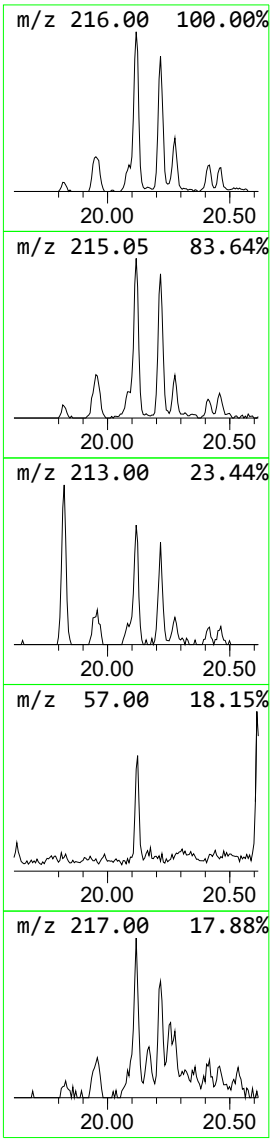
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.117	2.36 ng	107161	Chrysene-d12	21.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081523\
Data File : BG058734.D
Acq On : 15 Aug 2023 16:22
Operator : MA/JU
Sample : 04009-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CONC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
3-Hexen-2-one	4.306	34.8	ng	377113	1	7.808	216593	20.0
2-Pentanone, 4-...	4.911	43.4	ng	470044	1	7.808	216593	20.0
2,4,7,9-Tetrame...	13.342	17.9	ng	433745	3	14.453	485166	20.0
Anthracene, 2-m...	18.125	2.8	ng	86602	4	17.203	623124	20.0
4H-Cyclopenta[d...	18.278	3.2	ng	100085	4	17.203	623124	20.0
11H-Benzo[b]flu...	20.117	2.4	ng	107161	5	21.445	907453	20.0