LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.650	226	232	242	rVB	18329	27080	1.52%	0.200%
2	5.267	330	337	351	rBV	442801	702820	39.53%	5.187%
3	5.749	412	419	435	rBV	511398	847360	47.66%	6.253%
4	6.366	518	524	531	rBV	29005	45282	2.55%	0.334%
5	7.371	686	695	712	rBV	521636	932551	52.45%	6.882%
6	8.217	832	839	847	rBV	127991	218470	12.29%	1.612%
7	9.392	1031	1039	1052	rBV	319394	578370	32.53%	4.268%
8	11.049	1313	1321	1327	rBV	187207	335121	18.85%	2.473%
9	13.469	1726	1733	1740	rBV	809486	1243031	69.91%	9.173%
10	14.844	1960	1967	1973	rVV	320302	496321	27.91%	3.663%
11	14.909	1973	1978	1985	rVB	14586	24129	1.36%	0.178%
12	15.238	2029	2034	2041	rVB2	14497	21529	1.21%	0.159%
13	15.884	2138	2144	2154	rVB2	31128	46887	2.64%	0.346%
14	16.184	2189	2195	2201	rVB2	15043	23797	1.34%	0.176%
15	16.325	2212	2219	2237	rBV	734894	1166431	65.60%	8.608%
16	17.406	2397	2403	2408	rVB	12364	21743	1.22%	0.160%
17	17.582	2426	2433	2437	rBV	416108	630017	35.43%	4.649%
18	17.623	2437	2440	2447	rVB	203062	295689	16.63%	2.182%
19	17.717	2448	2456	2464	rBV	51686	97576	5.49%	0.720%
20	17.982	2495	2501	2508	rBV2	21375	39434	2.22%	0.291%
21	18.446	2575	2580	2586	rBV2	76744	152019	8.55%	1.122%
22	18.505	2586	2590	2595	rVB2	39233	63993	3.60%	0.472%
23	18.581	2599	2603	2608	rVB	15008	21967	1.24%	0.162%
24	18.652	2608	2615	2619	rBV2	48452	97327	5.47%	0.718%
25	18.945	2660	2665	2669	rBV	21615	31961	1.80%	0.236%
26	18.992	2669	2673	2680	rVB7	12106	19904	1.12%	0.147%
27	19.180	2701	2705	2710	rVB6	10901	18705	1.05%	0.138%
28	19.357	2729	2735	2740	rBV2	25691	50410	2.84%	0.372%
29	19.621	2774	2780	2786	rBV	329946	477885	26.88%	3.527%
30	19.709	2791	2795	2800	rVB4	18320	29666	1.67%	0.219%
31	19.950	2831	2836	2838	rBV2	52849	81635	4.59%	0.602%
32	19.985	2838	2842	2849	rVV	303955	426281	23.97%	3.146%
33	20.050	2849	2853	2857	rVB2	20853	31165	1.75%	0.230%
34	20.167	2867	2873	2878	rBV	1386349	1778089	100.00%	13.122%
35	20.303	2891	2896	2902	rVB4	22305	52865	2.97%	0.390%
36	20.467	2922	2924	2931	rVB	54543	64650	3.64%	0.477%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.567	2937	2941	2945	rBV	46610	58740	3.30%	0.433%
38	20.632	2949	2952	2955	rVB	26611	34465	1.94%	0.254%
39	20.767	2972	2975	2979	rBV	22944	31975	1.80%	0.236%
40	20.814	2980	2983	2986	rBV2	17890	26303	1.48%	0.194%
41	21.871	3154	3163	3168	rBV3	431072	934914	52.58%	6.899%
42	21.918	3168	3171	3179	rVB	119972	200483	11.28%	1.479%
43	24.175	3550	3555	3563	rBV	63871	190968	10.74%	1.409%
44	25.091	3706	3711	3726	rVB	78671	246819	13.88%	1.821%
45	25.261	3731	3740	3749	rVV2	218094	634097	35.66%	4.679%

Sum of corrected areas: 13550924

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
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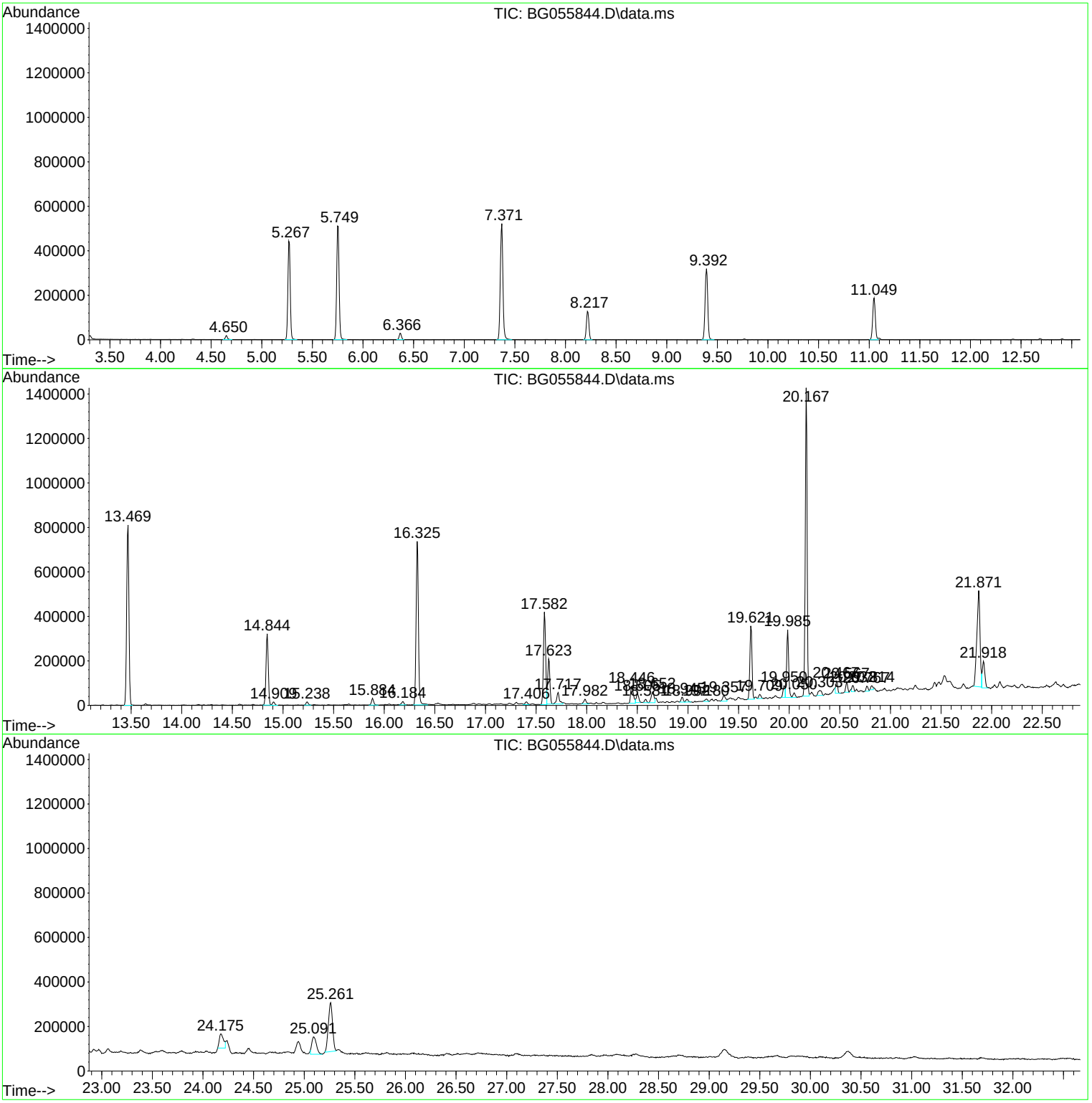
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

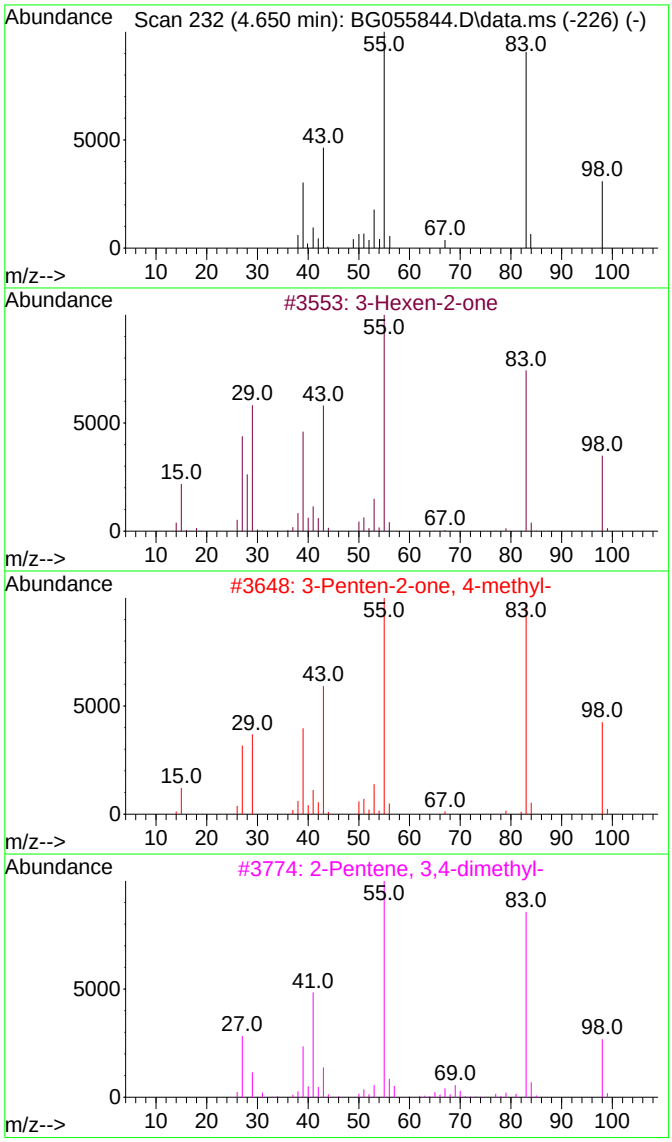
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

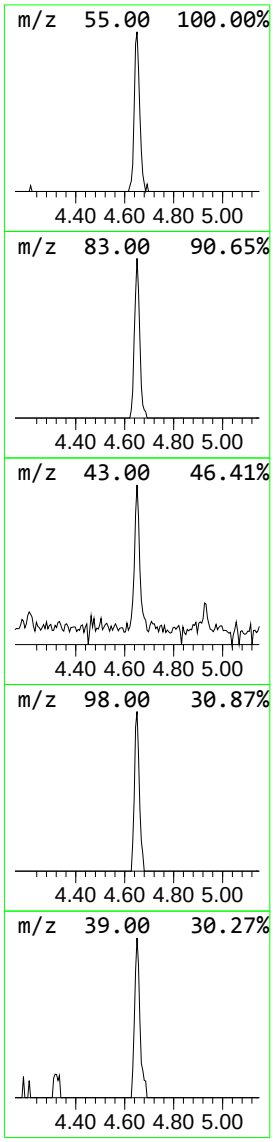
****

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.650	2.48 ng	27080	1,4-Dichlorobenzene-d4	8.217

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	87
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

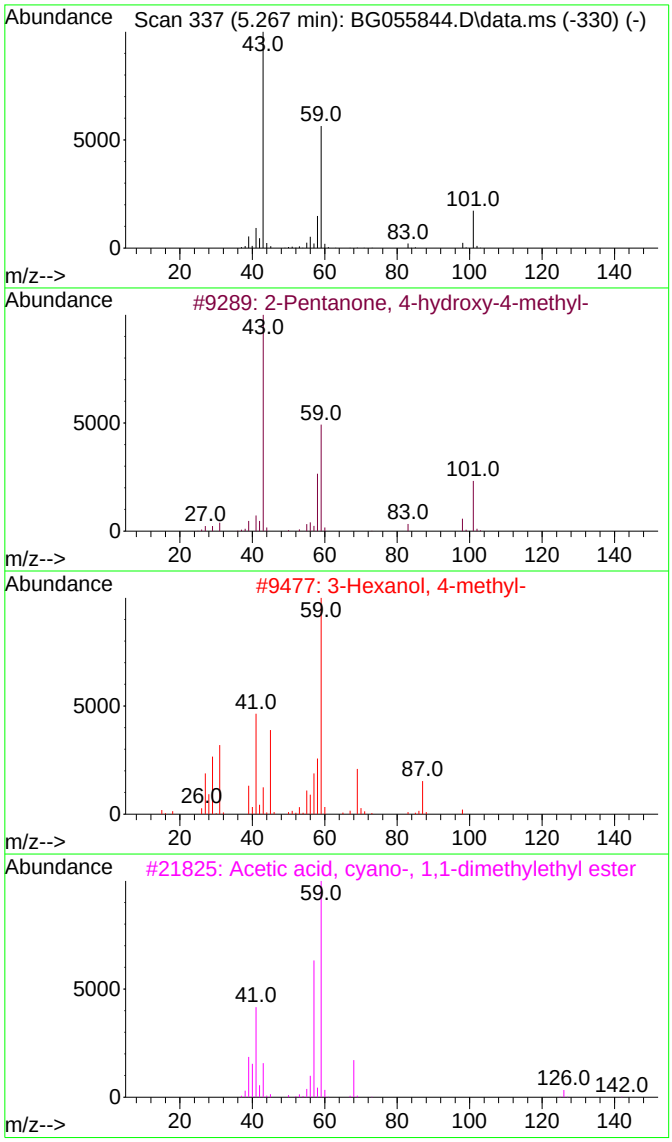
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

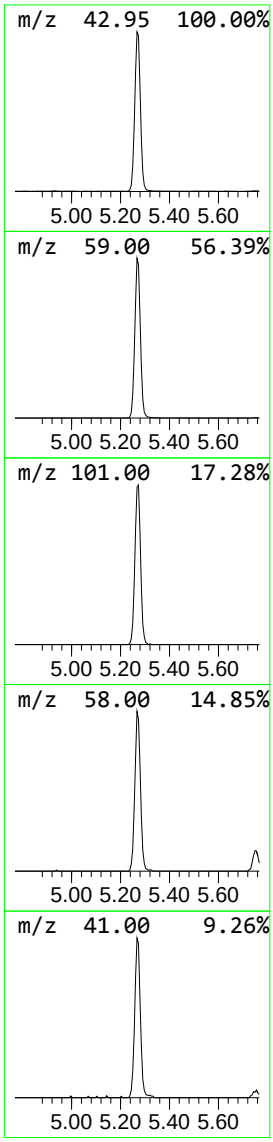
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.267	64.34 ng	702820	1,4-Dichlorobenzene-d4	8.217

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

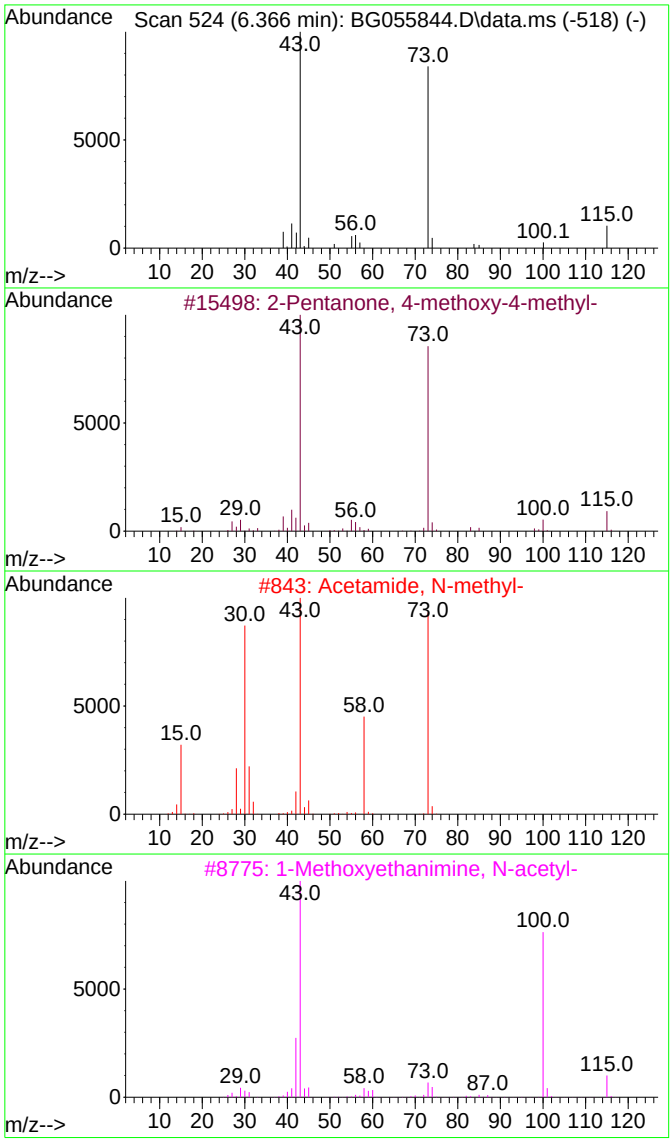
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

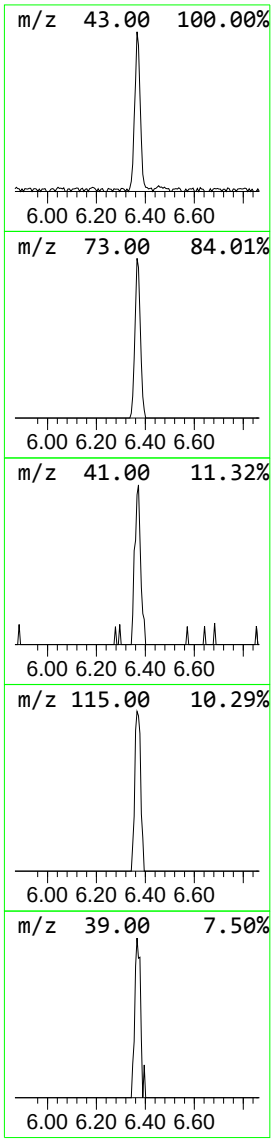
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.366	4.15 ng	45282	1,4-Dichlorobenzene-d4	8.217

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

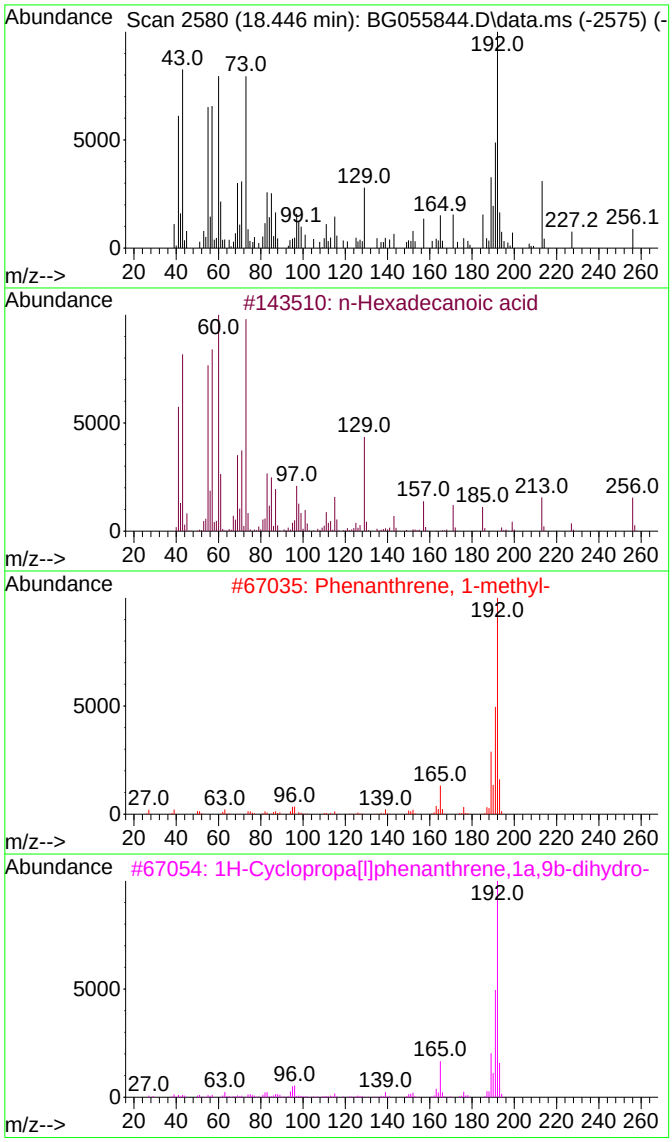
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

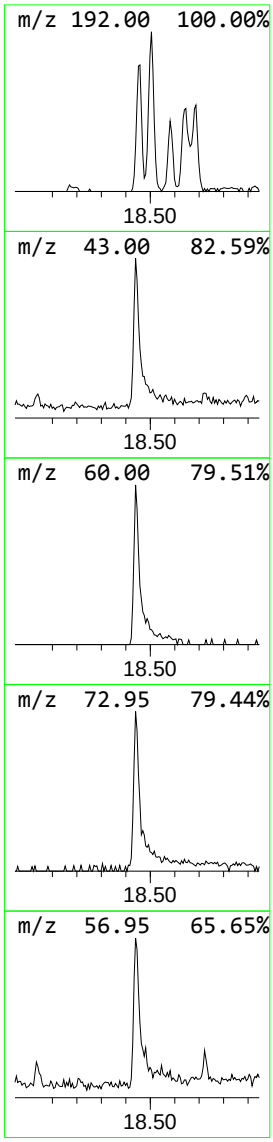
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	4.83 ng	152019	Phenanthrene-d10	17.582

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	70
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

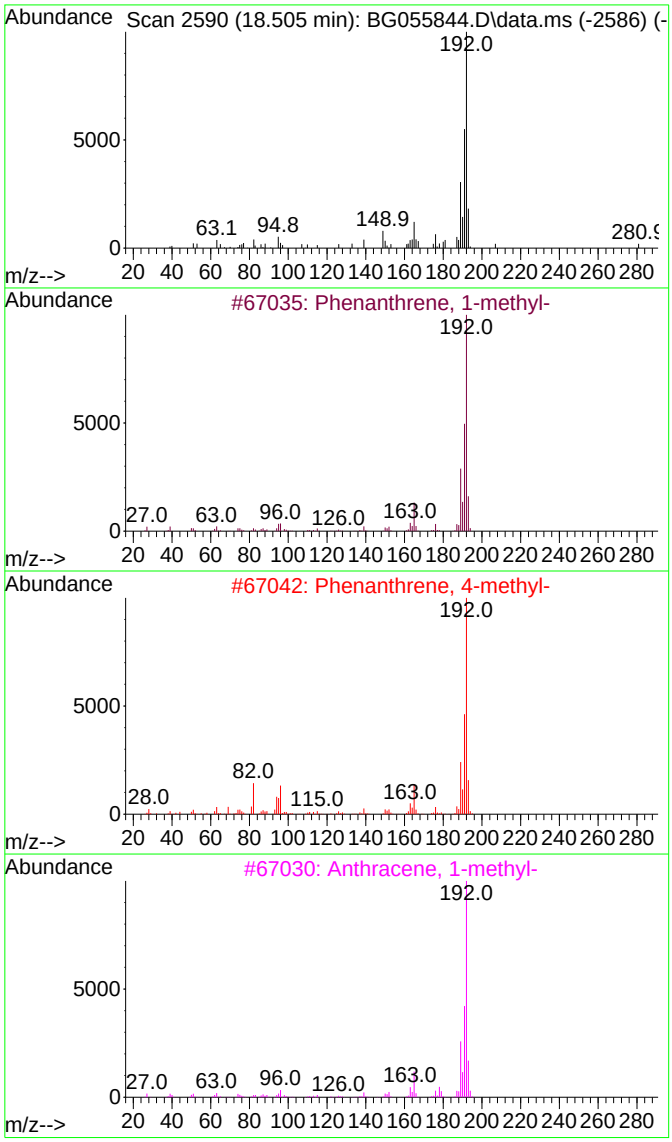
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

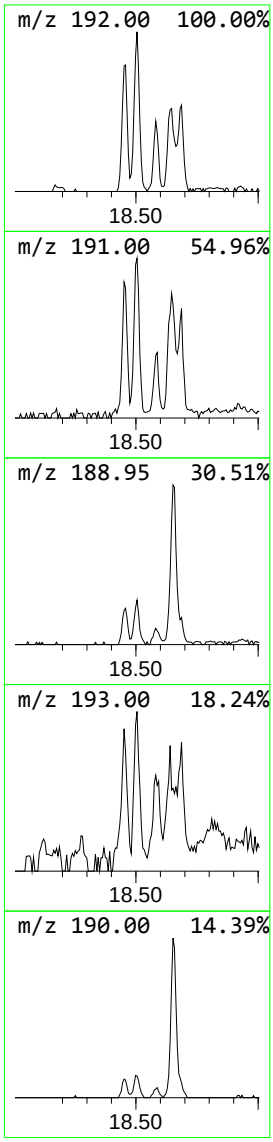
****

Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.505	2.03 ng	63993	Phenanthrene-d10	17.582

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

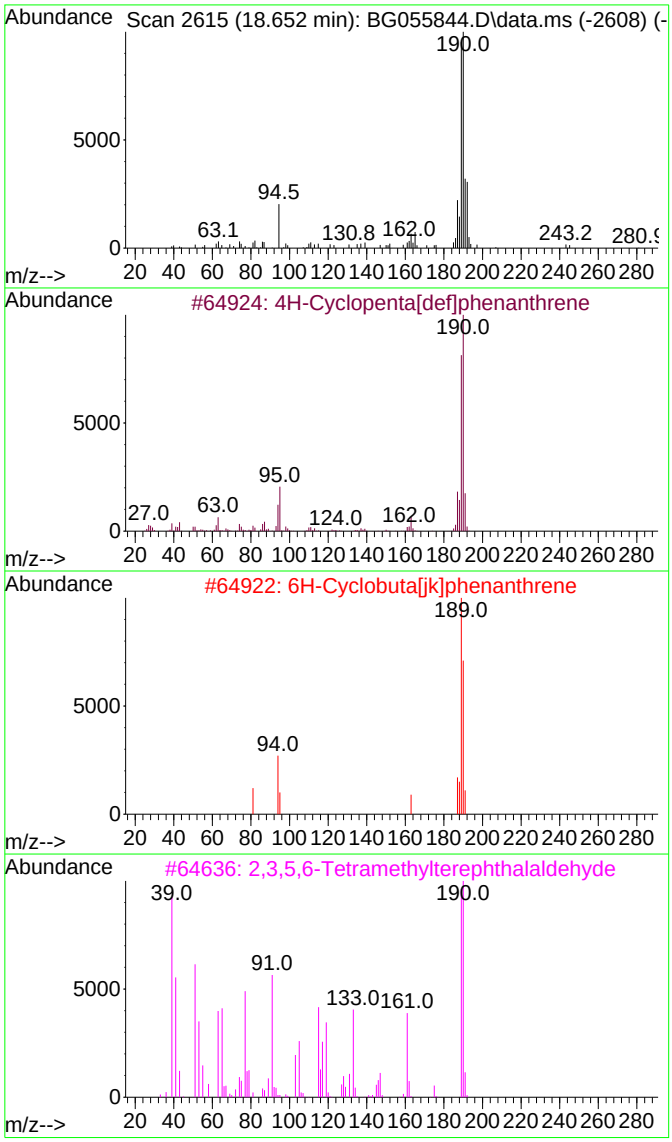
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

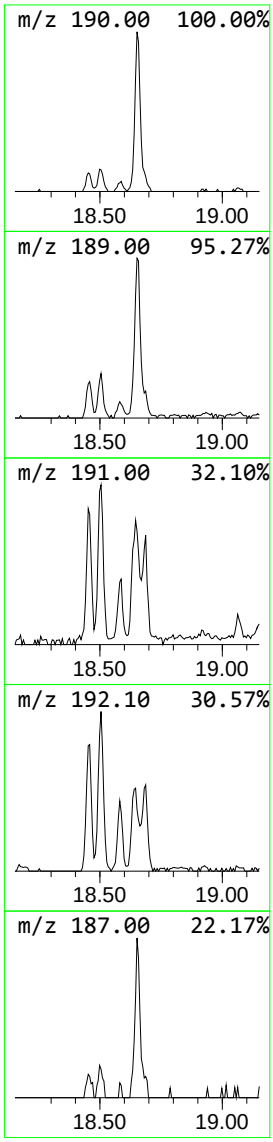
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.652	3.09 ng	97327	Phenanthrene-d10	17.582

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	40
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055844.D
Acq On : 30 Nov 2022 16:25
Operator : CG/JU
Sample : N5807-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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	4.650	2.5	ng	27080	1	8.217	218470	20.0
2-Pentanone, 4-...	5.267	64.3	ng	702820	1	8.217	218470	20.0
2-Pentanone, 4-...	6.366	4.2	ng	45282	1	8.217	218470	20.0
n-Hexadecanoic ...	18.446	4.8	ng	152019	4	17.582	630017	20.0
Phenanthrene, 1...	18.505	2.0	ng	63993	4	17.582	630017	20.0
4H-Cyclopenta[d...	18.652	3.1	ng	97327	4	17.582	630017	20.0