LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-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_M\Methods\8270-BM031325.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	320	326	334	rBV	1172035	1574370	12.51%	1.752%
2	5.369	399	405	418	rBV	4954144	6888995	54.73%	7.665%
3	5.981	504	509	517	rBV	197519	290715	2.31%	0.323%
4	6.957	668	675	691	rBV	4842575	7346437	58.36%	8.174%
5	7.786	806	816	823	rVB	1281151	1925171	15.29%	2.142%
6	8.939	1003	1012	1021	rBV	2744360	4347136	34.54%	4.837%
7	10.580	1283	1291	1298	rBV	1489721	2418025	19.21%	2.690%
8	13.051	1703	1711	1728	rBV	6454867	9051345	71.91%	10.070%
9	14.427	1936	1945	1951	rBV	2246395	3120400	24.79%	3.472%
10	15.786	2170	2176	2182	rVB	829550	1106962	8.79%	1.232%
11	15.915	2191	2198	2208	rBV	6127589	8143553	64.70%	9.060%
12	17.168	2405	2411	2415	rBV	2609334	3489788	27.73%	3.883%
13	17.209	2415	2418	2425	rVB	435833	564167	4.48%	0.628%
14	17.298	2430	2433	2439	rVB	144408	193738	1.54%	0.216%
15	18.045	2555	2560	2561	rBV	124564	155253	1.23%	0.173%
16	18.068	2561	2564	2574	rVB2	411230	811366	6.45%	0.903%
17	18.239	2587	2593	2597	rBV2	255300	482079	3.83%	0.536%
18	18.274	2597	2599	2606	rVB	123479	147299	1.17%	0.164%
19	18.962	2712	2716	2721	rBV3	110286	164940	1.31%	0.184%
20	19.097	2735	2739	2748	rBV2	97948	199213	1.58%	0.222%
21	19.227	2756	2761	2768	rVB	1435611	1840932	14.63%	2.048%
22	19.350	2775	2782	2790	rBV5	138926	275063	2.19%	0.306%
23	19.586	2813	2822	2831	rBV	2177707	3313121	26.32%	3.686%
24	19.662	2832	2835	2842	rVB3	72505	136995	1.09%	0.152%
25	19.792	2852	2857	2862	rBV	10959866	12587071	100.00%	14.004%
26	19.921	2874	2879	2884	rBV4	132101	281540	2.24%	0.313%
27	20.086	2903	2907	2911	rVB	281823	389213	3.09%	0.433%
28	20.186	2920	2924	2928	rBV	210881	271902	2.16%	0.303%
29	20.244	2930	2934	2937	rVV	258098	364634	2.90%	0.406%
30	20.380	2954	2957	2961	rBV2	195338	262595	2.09%	0.292%
31	20.427	2961	2965	2969	rVV	236571	288290	2.29%	0.321%
32	21.009	3061	3064	3067	rVB	138053	166712	1.32%	0.185%
33	21.050	3068	3071	3074	rVB	162110	174312	1.38%	0.194%
34	21.091	3074	3078	3083	rBV2	347009	548861	4.36%	0.611%
35	21.403	3123	3131	3135	rBV2	3146450	5922979	47.06%	6.590%
36	21.444	3135	3138	3147	rVB	976782	1502189	11.93%	1.671%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-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_M\Methods\8270-BM031325.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.591	3160	3163	3170	rVB2	178817	291416	2.32%	0.324%
38	23.456	3474	3480	3487	rBV	688395	1983008	15.75%	2.206%
39	24.127	3589	3594	3606	rVB	526711	1269717	10.09%	1.413%
40	24.262	3610	3617	3625	rVV	754916	1805724	14.35%	2.009%
41	24.403	3634	3641	3648	rBV	1602760	3783251	30.06%	4.209%

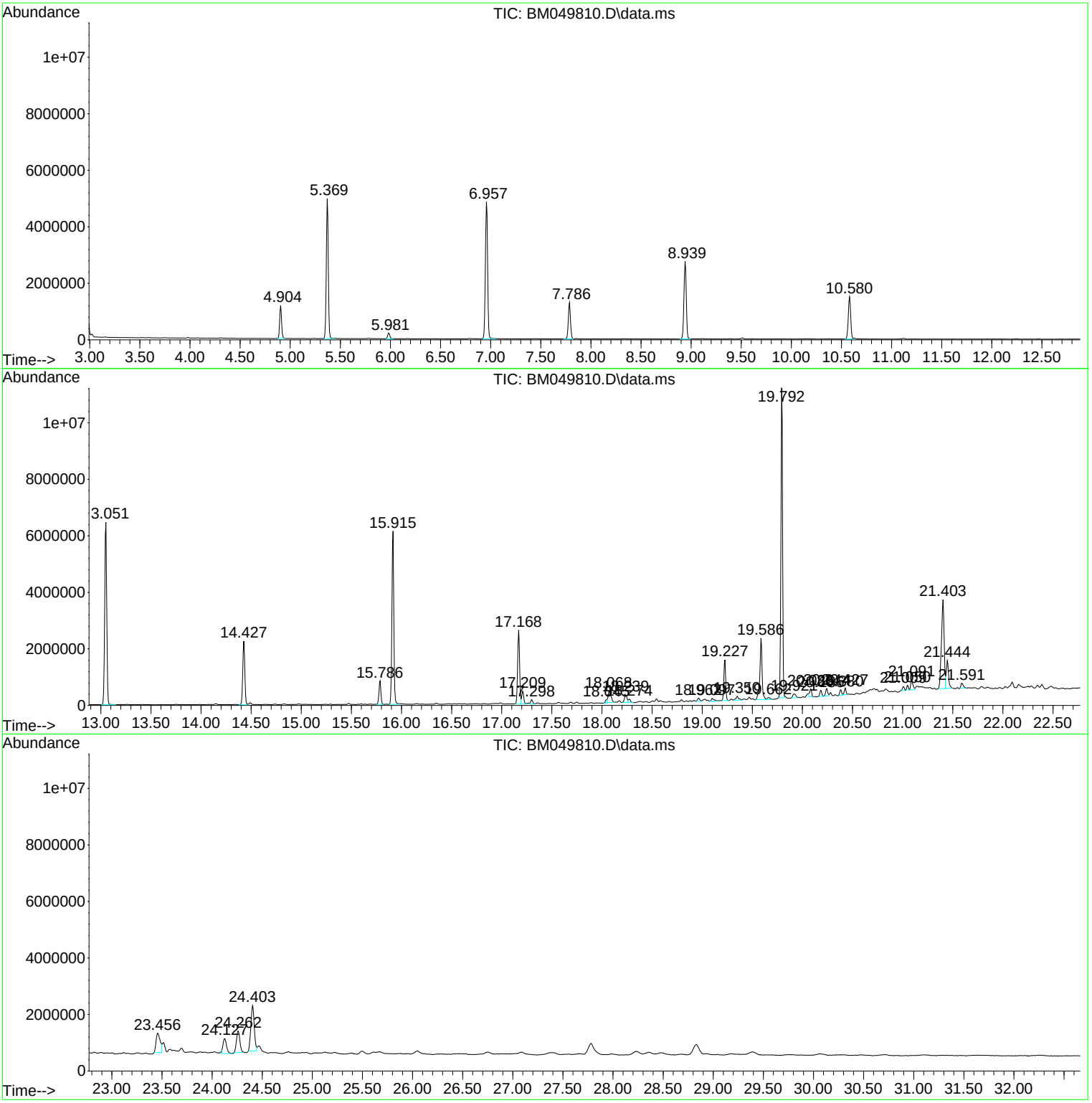
Sum of corrected areas: 89880477

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

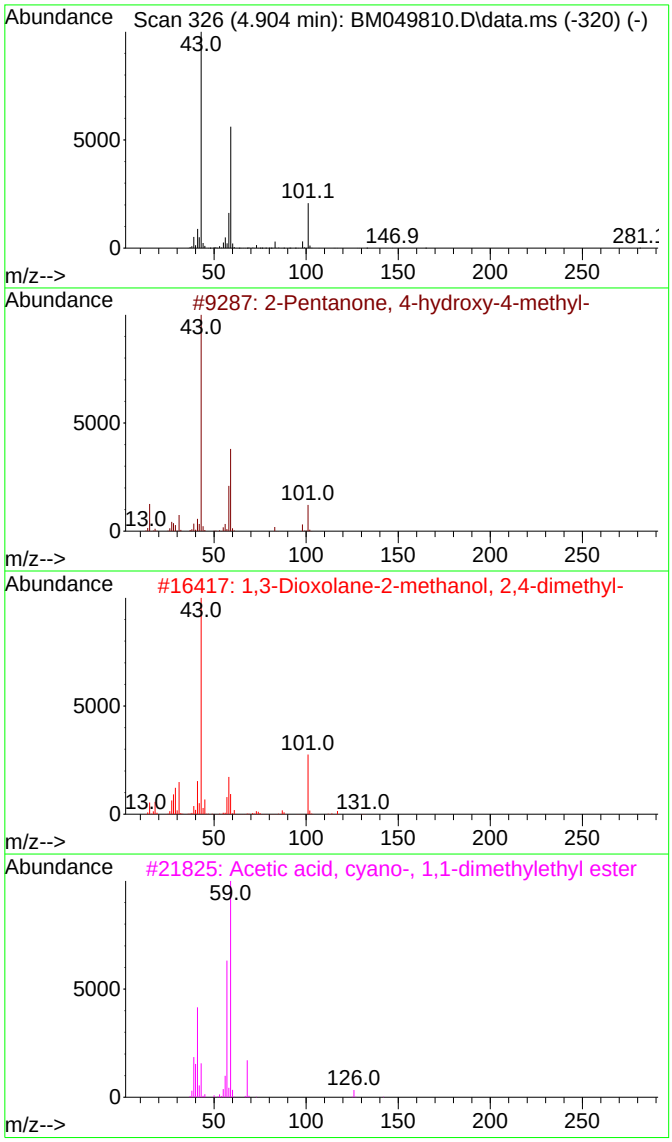
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

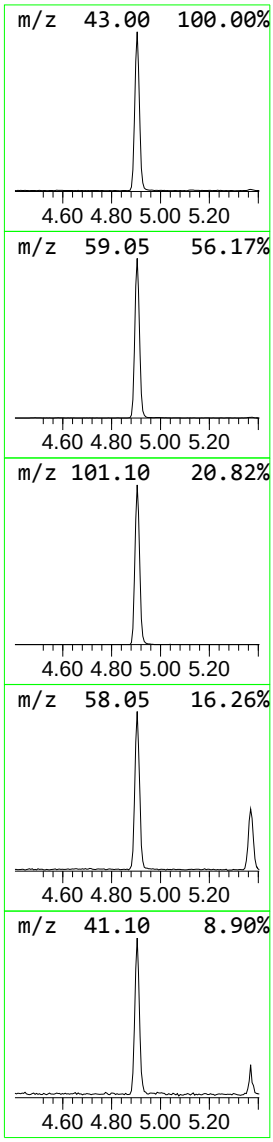
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	16.36 ng	1574370	1,4-Dichlorobenzene-d4	7.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

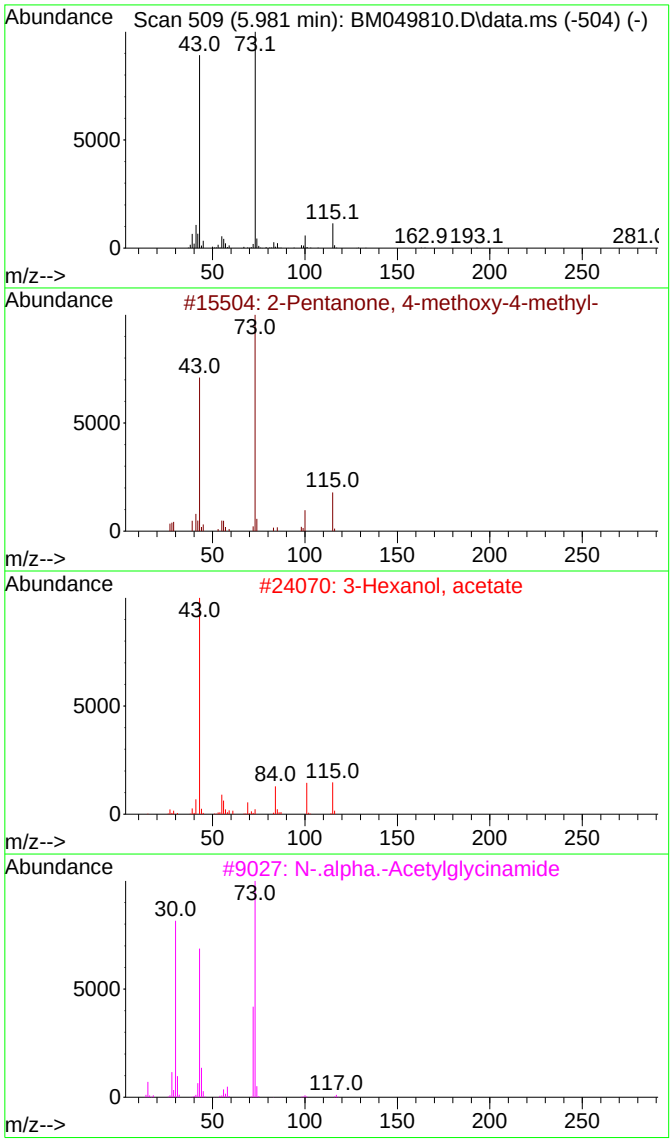
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

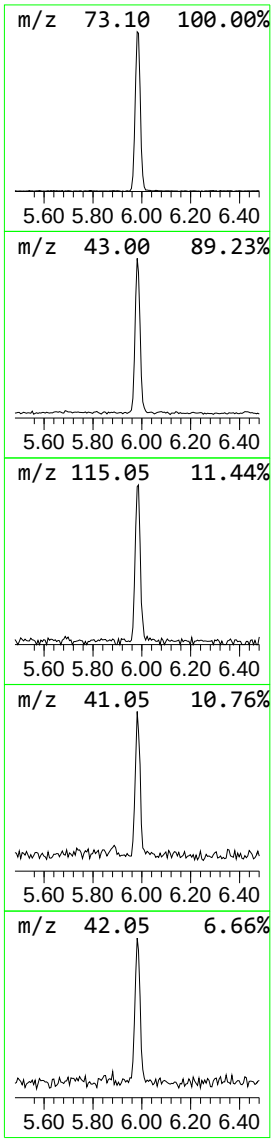
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	3.02 ng	290715	1,4-Dichlorobenzene-d4	7.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	32
3	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4	3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

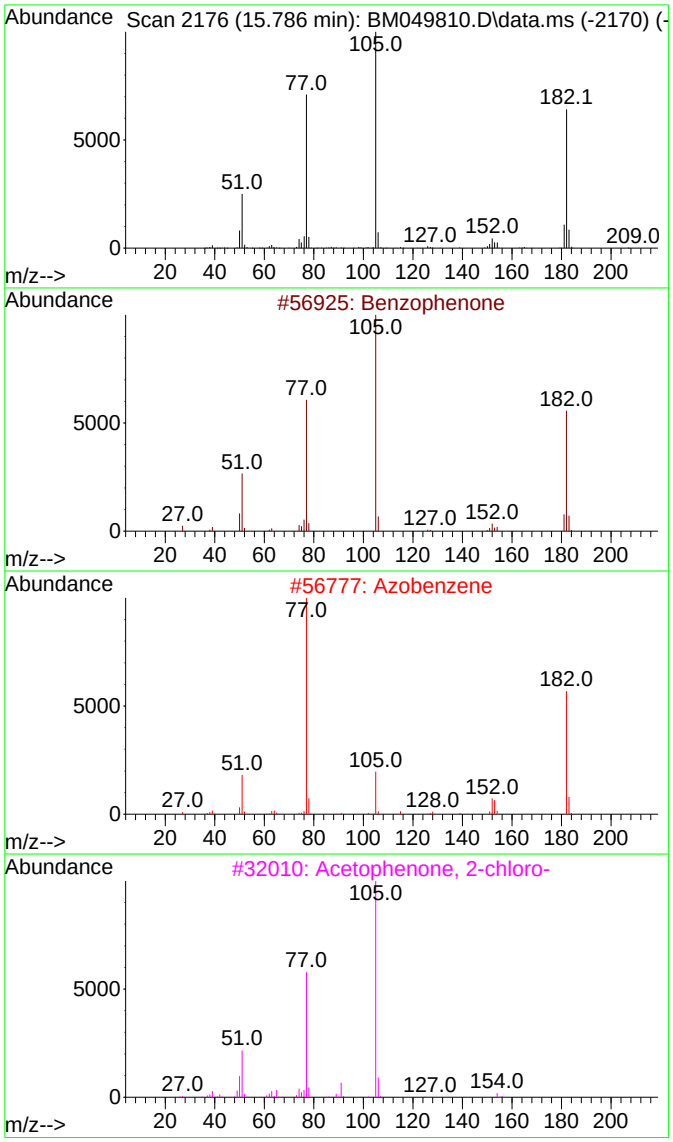
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

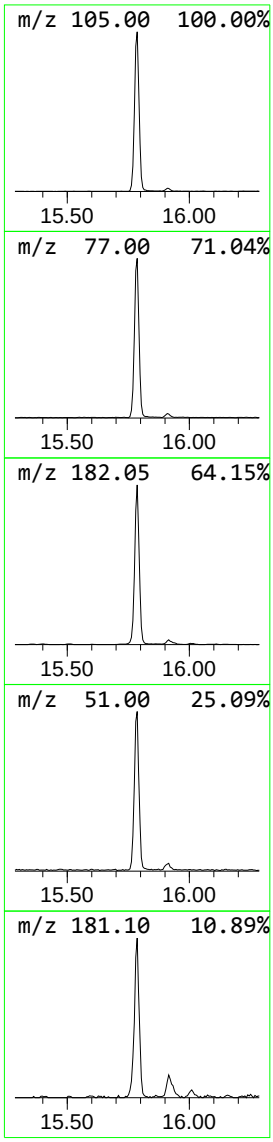
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	7.09 ng	1106960	Acenaphthene-d10	14.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

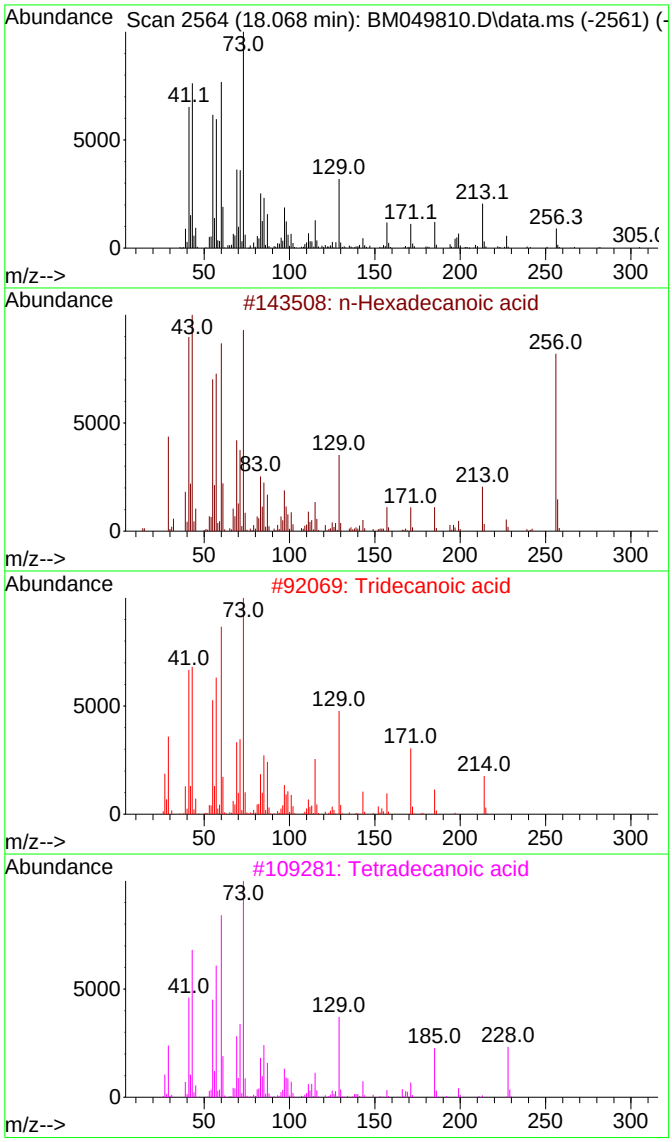
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

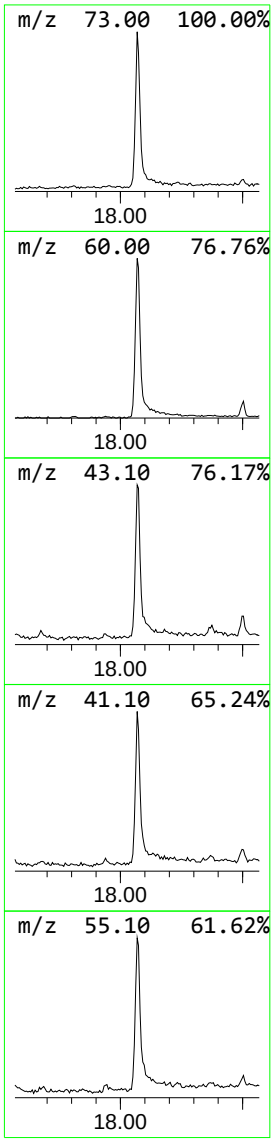
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	4.65 ng	811366	Phenanthrene-d10	17.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TT-3

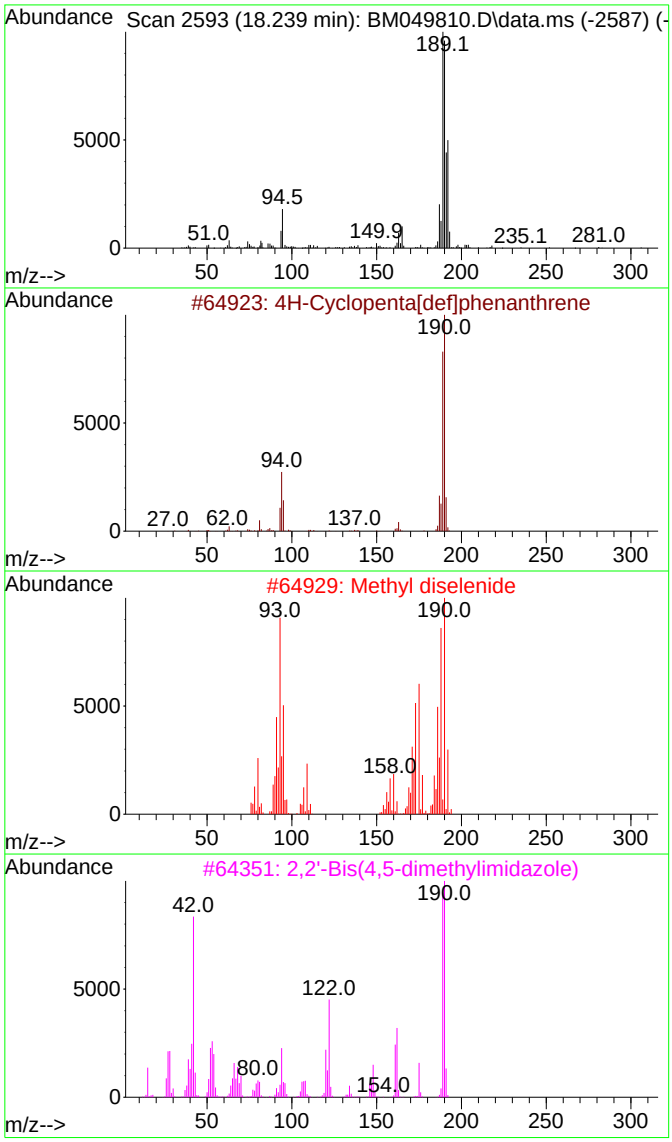
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

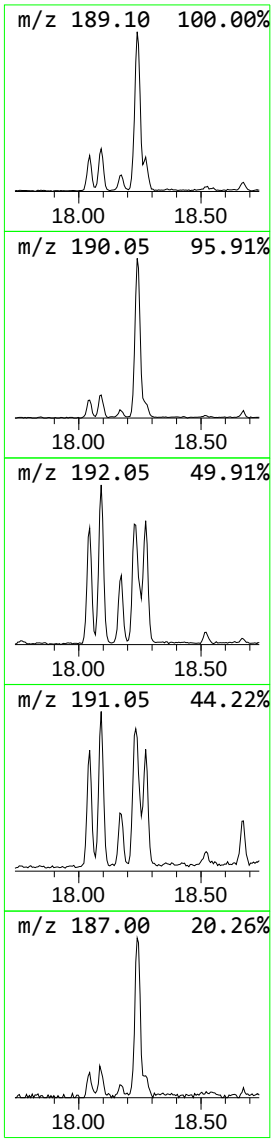
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	2.76 ng	482079	Phenanthrene-d10	17.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Methyl diselenide	190	C2H6Se2	007101-31-7	41
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35
5	Propanoic acid, 2-(2,4-dichlorop...	378	C15H10Cl4O3	284488-02-4	20





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Operator : RC/JU
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Misc :
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

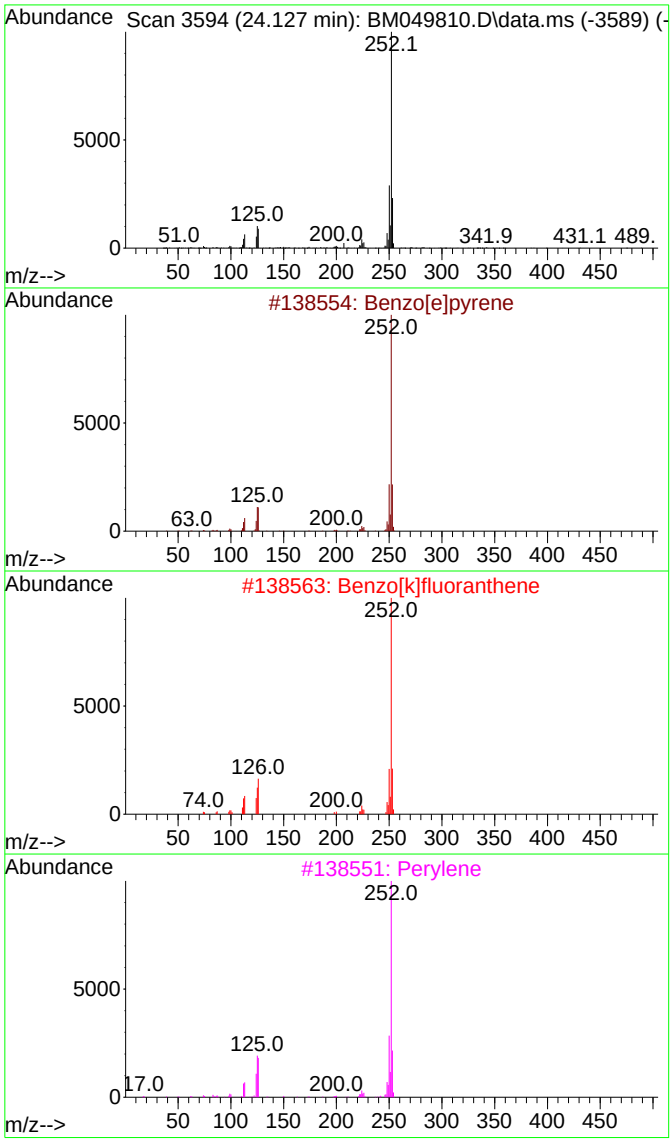
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

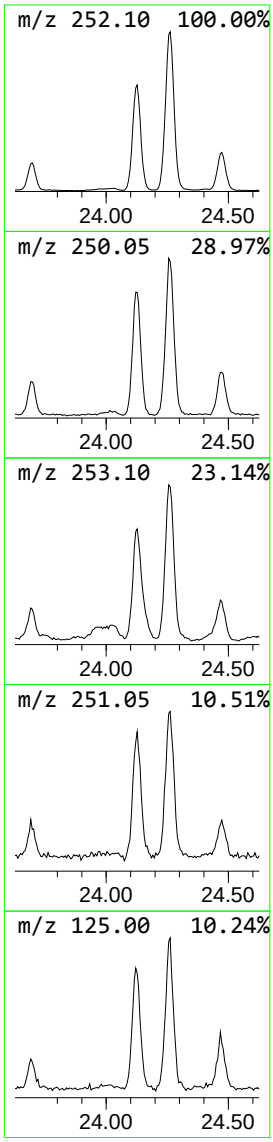
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.127	6.71 ng	1269720	Perylene-d12	24.403

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049810.D
Acq On : 03 Apr 2025 17:53
Operator : RC/JU
Sample : Q1695-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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
2-Pentanone, 4-...	4.904	16.4	ng	1574370	1	7.786	1925170	20.0
2-Pentanone, 4-...	5.981	3.0	ng	290715	1	7.786	1925170	20.0
Benzophenone	15.786	7.1	ng	1106960	3	14.427	3120400	20.0
n-Hexadecanoic ...	18.068	4.7	ng	811366	4	17.168	3489790	20.0
4H-Cyclopenta[d...	18.239	2.8	ng	482079	4	17.168	3489790	20.0
Benzo[e]pyrene	24.127	6.7	ng	1269720	6	24.403	3783250	20.0