LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

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-BG030525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	317	324	331	rBV	100402	165990	11.61%	1.033%
2	5.456	396	403	410	rBV	382688	647811	45.32%	4.031%
3	6.061	502	506	513	rVB2	15600	24145	1.69%	0.150%
4	7.031	663	671	681	rBV	416900	725441	50.75%	4.514%
5	7.865	806	813	820	rBV	179515	310262	21.71%	1.931%
6	9.011	998	1008	1015	rBV	276228	467092	32.68%	2.906%
7	9.093	1018	1022	1028	rVB3	13469	20400	1.43%	0.127%
8	10.650	1279	1287	1294	rBV	258776	468519	32.78%	2.915%
9	11.690	1457	1464	1469	rBV3	11196	24242	1.70%	0.151%
10	12.084	1526	1531	1537	rBV	26003	40831	2.86%	0.254%
11	13.035	1689	1693	1699	rVB5	10684	16575	1.16%	0.103%
12	13.106	1699	1705	1713	rVB	617727	958222	67.04%	5.962%
13	13.323	1736	1742	1749	rBV2	24357	37086	2.59%	0.231%
14	14.205	1888	1892	1902	rBV	19926	46775	3.27%	0.291%
15	14.398	1920	1925	1930	rVB3	24950	33462	2.34%	0.208%
16	14.487	1930	1940	1947	rBV	372395	613832	42.94%	3.819%
17	14.545	1947	1950	1956	rVB4	13022	20944	1.47%	0.130%
18	14.886	2005	2008	2015	rVB6	9555	20693	1.45%	0.129%
19	15.350	2082	2087	2092	rBV3	22140	32737	2.29%	0.204%
20	15.532	2113	2118	2119	rBV4	13577	16526	1.16%	0.103%
21	15.844	2164	2171	2178	rVB	167674	257100	17.99%	1.600%
22	15.967	2186	2192	2201	rBV	532415	816850	57.15%	5.083%
23	16.214	2229	2234	2236	rBV5	22315	31991	2.24%	0.199%
24	16.402	2263	2266	2272	rVB2	28821	44542	3.12%	0.277%
25	16.584	2294	2297	2301	rBV6	13881	16100	1.13%	0.100%
26	17.054	2373	2377	2386	rVB7	25667	45953	3.21%	0.286%
27	17.225	2400	2406	2410	rBV2	445633	665478	46.56%	4.141%
28	17.266	2410	2413	2420	rVB	200121	269811	18.88%	1.679%
29	17.354	2425	2428	2433	rVB	60227	88234	6.17%	0.549%
30	17.407	2433	2437	2443	rBV9	21066	45033	3.15%	0.280%
31	17.612	2469	2472	2478	rBV6	38696	63910	4.47%	0.398%
32	18.100	2551	2555	2556	rBV	43972	49077	3.43%	0.305%
33	18.129	2556	2560	2568	rVB2	148647	292611	20.47%	1.821%
34	18.300	2583	2589	2592	rBV3	87359	160759	11.25%	1.000%
35	18.558	2630	2633	2637	rVB3	42445	50289	3.52%	0.313%
36	18.599	2637	2640	2643	rVV3	28347	36252	2.54%	0.226%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

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-BG030525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.635	2643	2646	2653	rVB7	36433	60700	4.25%	0.378%
38	19.152	2730	2734	2739	rBV	54350	93854	6.57%	0.584%
39	19.281	2750	2756	2761	rBV	876854	1196708	83.72%	7.446%
40	19.639	2808	2817	2826	rBV	808277	1304435	91.26%	8.117%
41	19.845	2847	2852	2856	rVB	970852	1165526	81.54%	7.252%
42	20.133	2899	2901	2905	rVB	106600	117907	8.25%	0.734%
43	20.233	2915	2918	2922	rVB2	67510	86638	6.06%	0.539%
44	21.138	3069	3072	3078	rVB3	115792	191979	13.43%	1.195%
45	21.455	3119	3126	3131	rBV2	578020	1429355	100.00%	8.894%
46	21.502	3131	3134	3147	rVB	360253	602937	42.18%	3.752%
47	21.643	3155	3158	3163	rBV2	75192	131692	9.21%	0.819%
48	23.535	3473	3480	3486	rBV2	280657	820685	57.42%	5.107%
49	24.340	3612	3617	3625	rVB	250256	572253	40.04%	3.561%
50	24.481	3634	3641	3647	rBV3	256828	671075	46.95%	4.176%

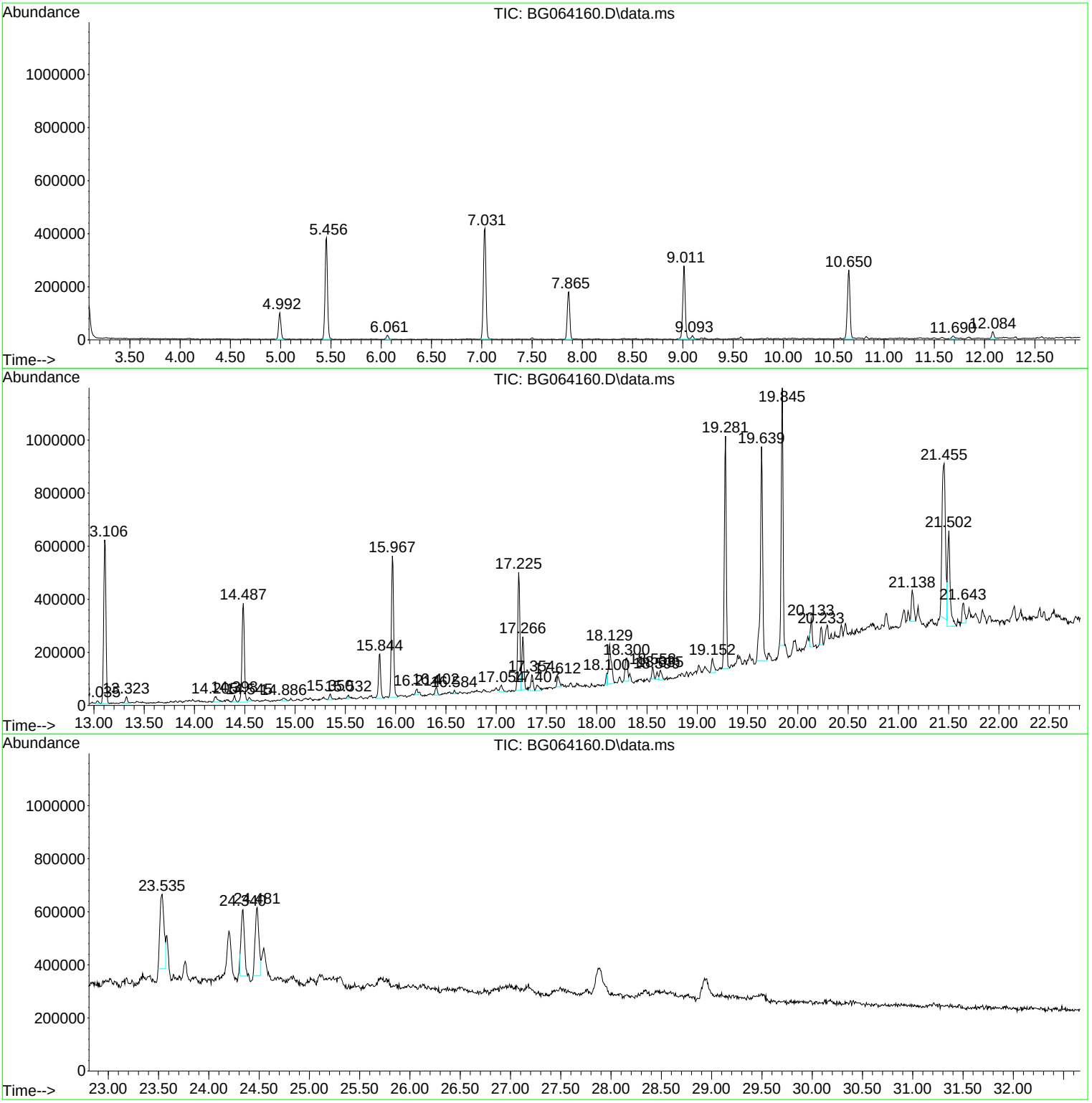
Sum of corrected areas: 16071319

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

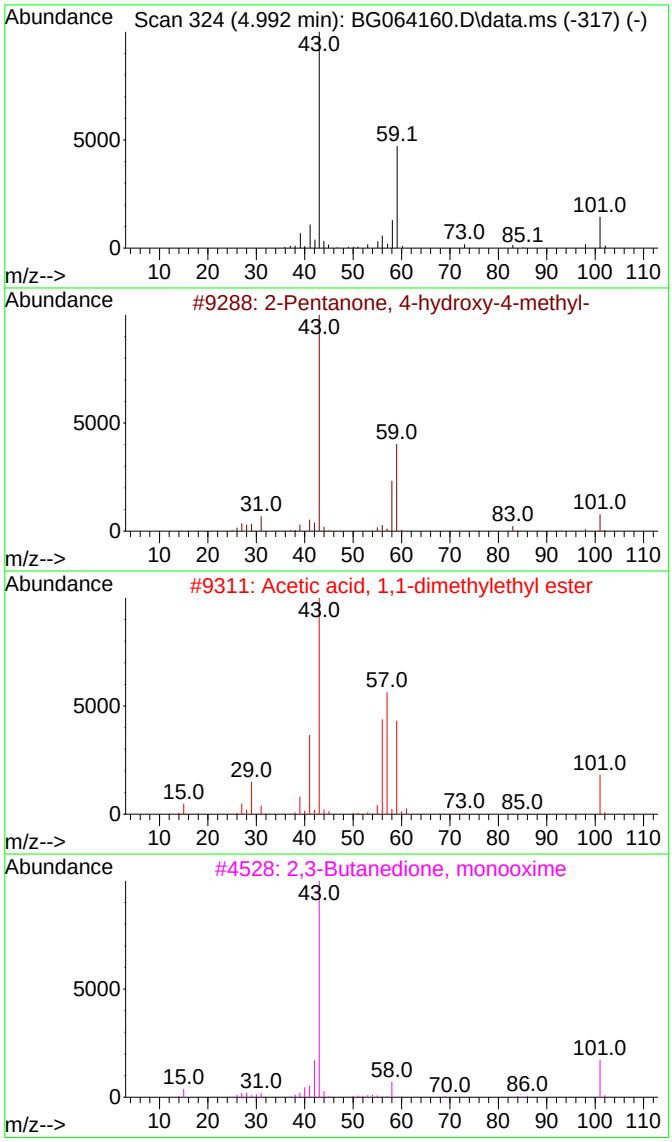
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

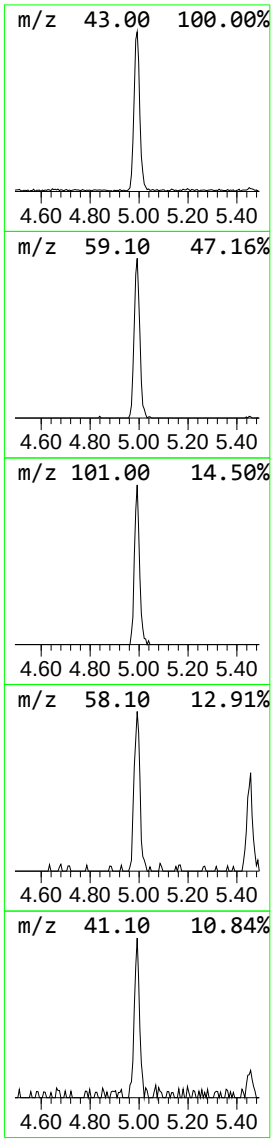
****

Peak Number 1 unknown4.992 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	10.70 ng	165990	1,4-Dichlorobenzene-d4	7.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

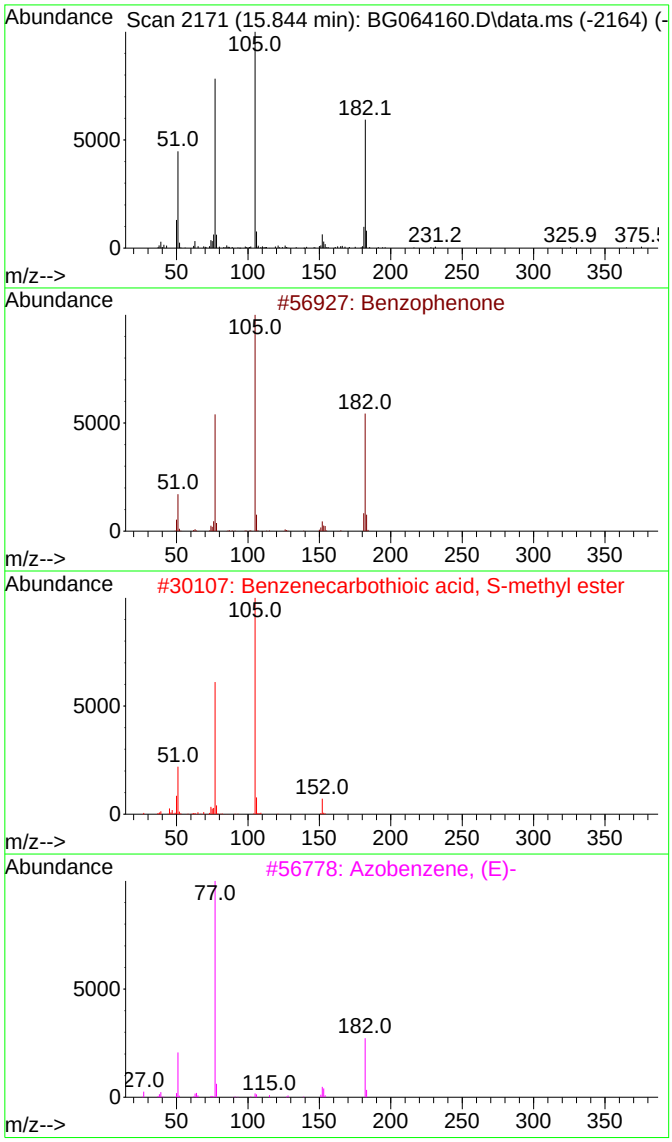
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

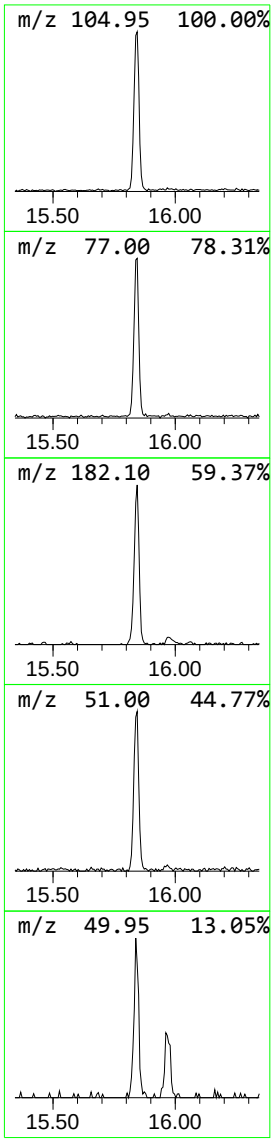
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.844	8.38 ng	257100	Acenaphthene-d10	14.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	68
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	64
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	58
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

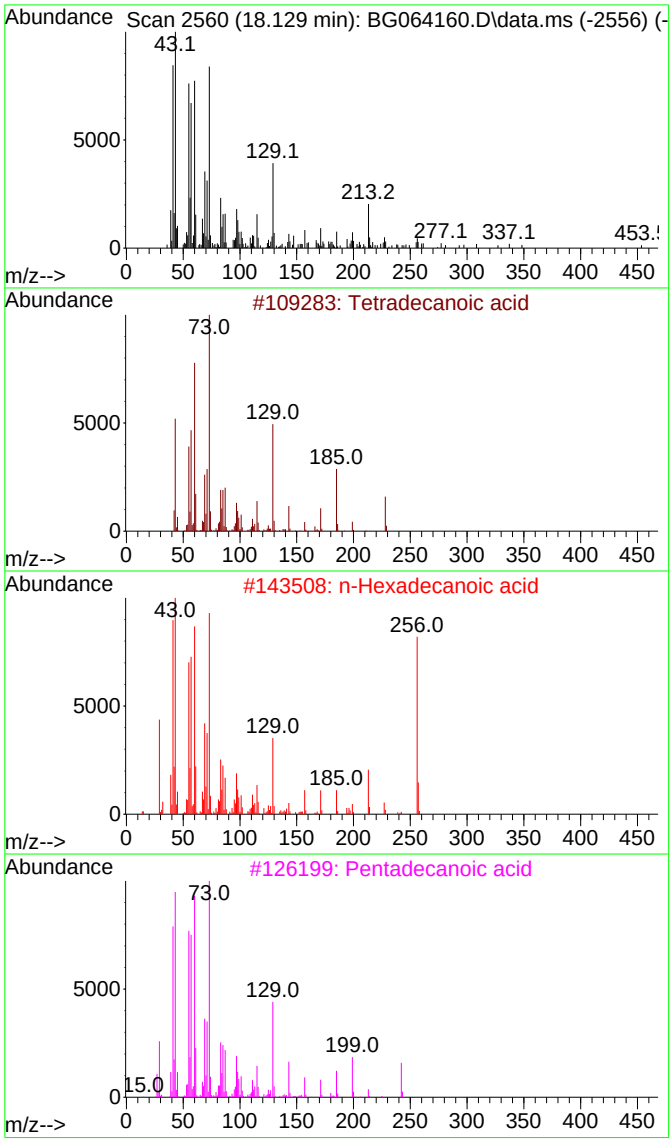
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

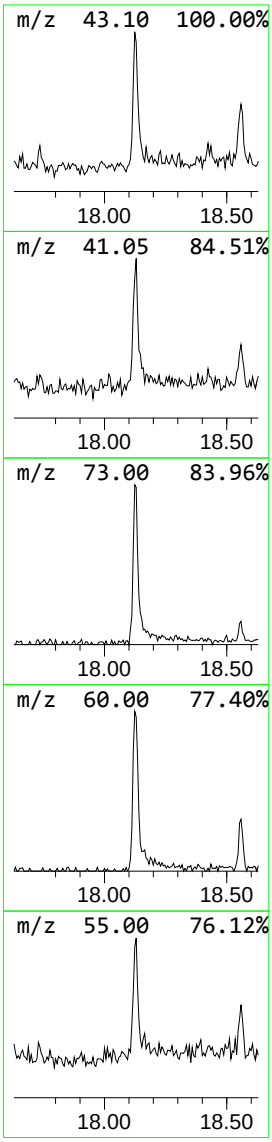
****

Peak Number 3 Tetradecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.129	8.79 ng	292611	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

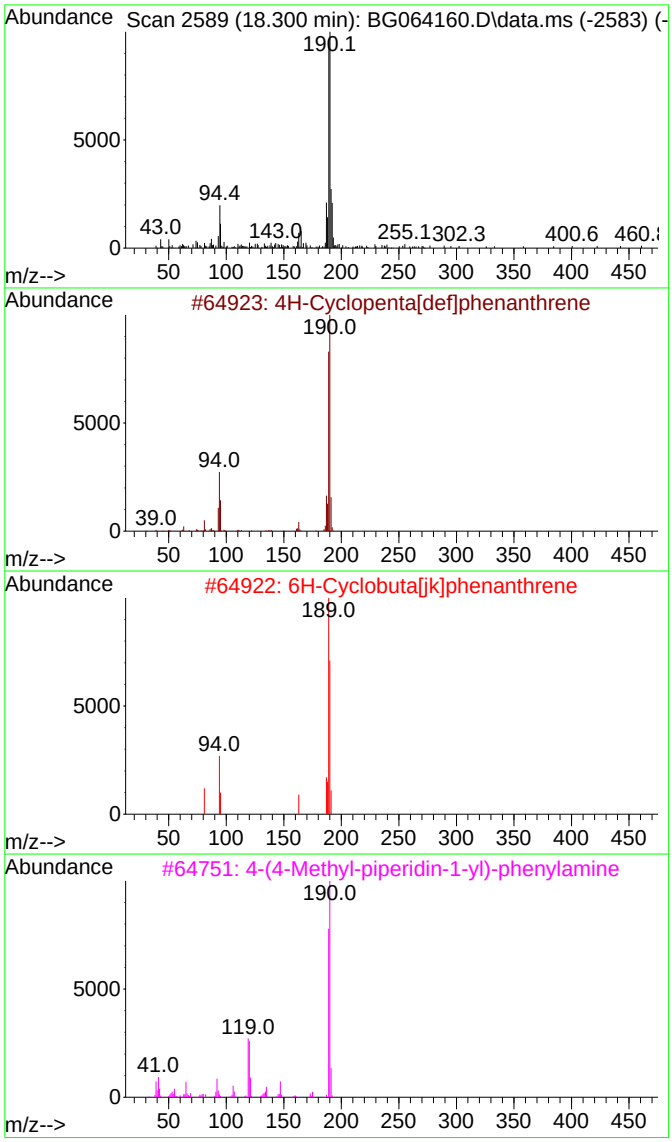
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

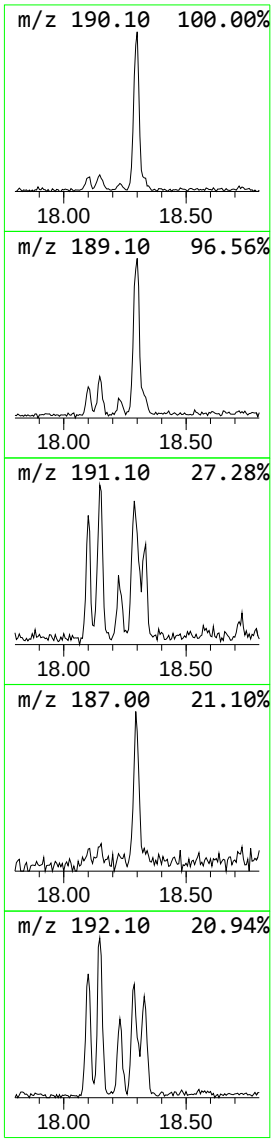
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.300	4.83 ng	160759	Phenanthrene-d10	17.225

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	64
3	4-(4-Methyl-piperidin-1-yl)-phen...	190	C12H18N2	342013-25-6	50
4	Benzo[1,2-b:3,4-b']dithiophene	190	C10H6S2	000211-02-9	30
5	Benzo[1,2-b:4,3-b']dithiophene	190	C10H6S2	000210-80-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

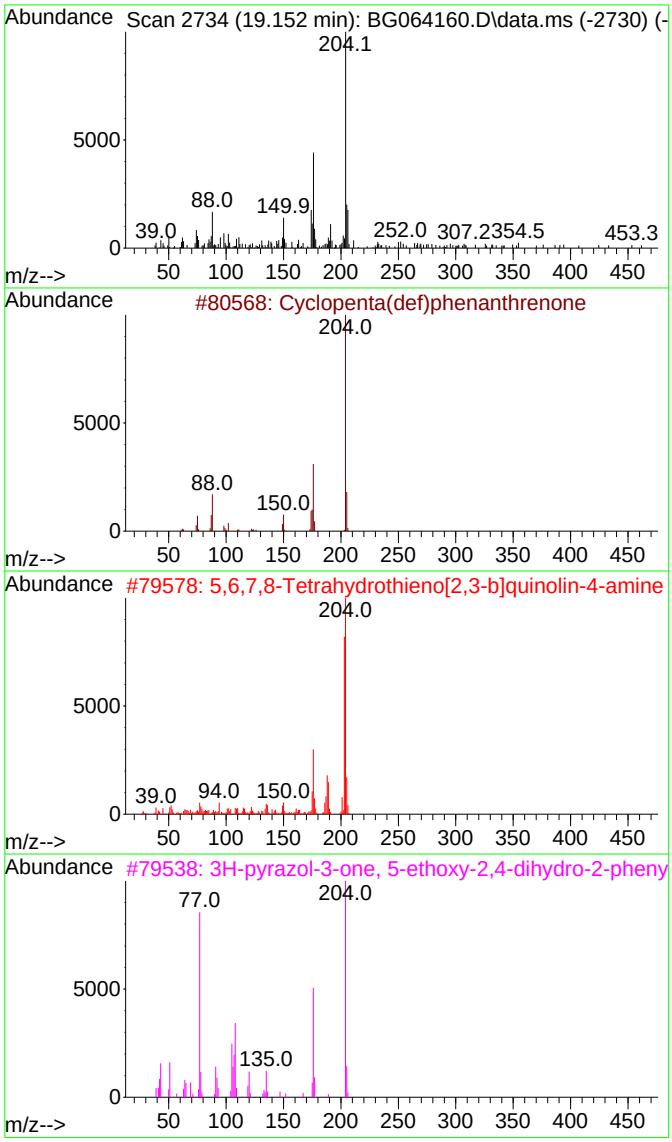
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

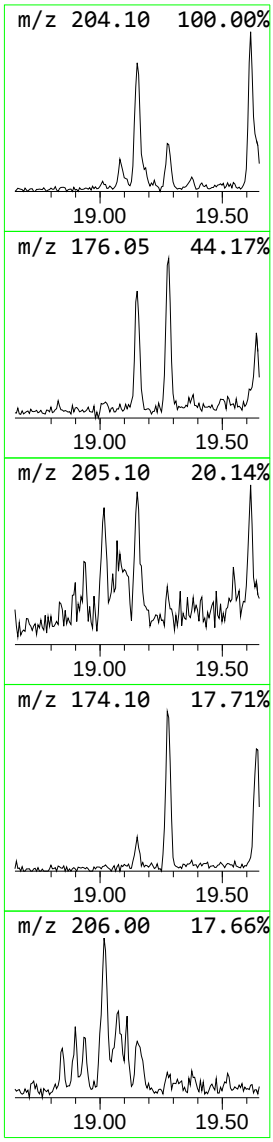
****

Peak Number 5 Cyclopenta(def)phenanthrenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.152	2.82 ng	93854	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	87
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	80
3	3H-pyrazol-3-one, 5-ethoxy-2,4-d...	204	C11H12N2O2	1000400-47-1	64
4	Etilefrin, N-pentafluoropropiony...	619	C19H12F15NO5	1000417-50-7	59
5	Shikimic acid, 4TMS	462	C19H42O5Si4	055520-78-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

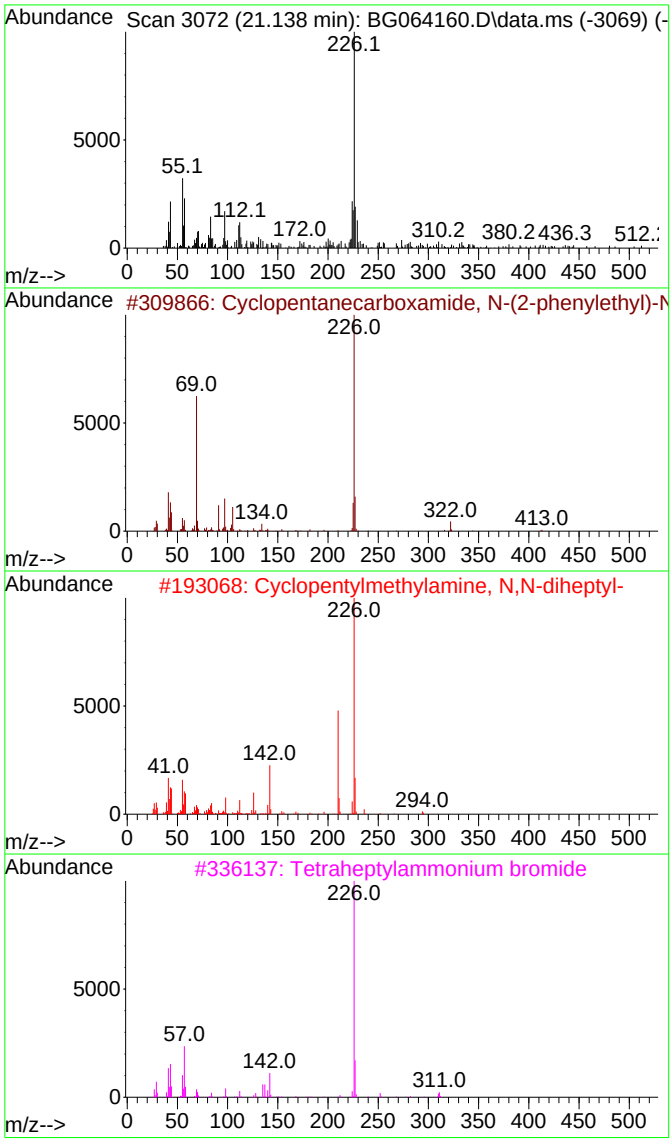
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

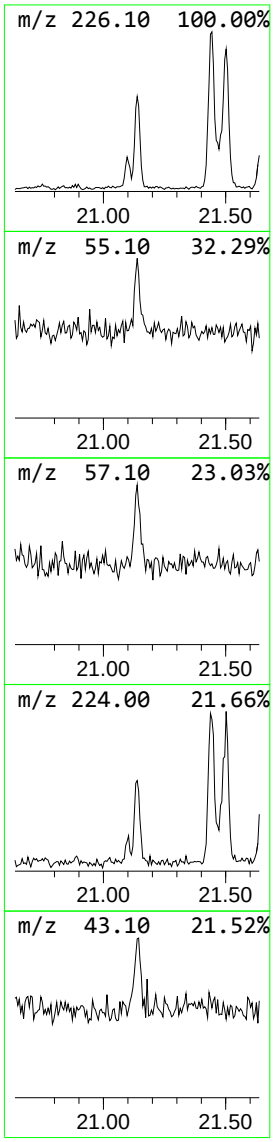
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentanecarboxamide, N-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.138	2.69 ng	191979	Chrysene-d12	21.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxamide, N-(2-ph...	413	C28H47NO	1000451-59-7	59
2	Cyclopentylmethylamine, N,N-dihe...	295	C20H41N	1000310-50-0	59
3	Tetraheptylammonium bromide	489	C28H60BrN	004368-51-8	59
4	benzenamine, 4-(2-benzothiazolyl)-	226	C13H10N2S	1000400-93-4	59
5	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064160.D
Acq On : 2 Apr 2025 19:44
Operator : RC/JU
Sample : Q1686-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EO-03-040125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.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
unknown4.992	4.992	10.7	ng	165990	1	7.865	310262	20.0
Benzophenone	15.844	8.4	ng	257100	3	14.487	613832	20.0
Tetradecanoic acid	18.129	8.8	ng	292611	4	17.225	665478	20.0
4H-Cyclopenta[d...	18.300	4.8	ng	160759	4	17.225	665478	20.0
Cyclopenta(def)...	19.152	2.8	ng	93854	4	17.225	665478	20.0
Cyclopentanecar...	21.138	2.7	ng	191979	5	21.455	1429360	20.0