LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.188	317	323	331	rBV	28323	45559	2.65%	0.348%
2	5.669	398	405	420	rBV	454536	772138	44.94%	5.904%
3	7.291	673	681	696	rBV	461614	828192	48.20%	6.332%
4	8.125	817	823	837	rVB	133832	234097	13.63%	1.790%
5	9.306	1016	1024	1036	rBV	287140	515795	30.02%	3.944%
6	10.705	1255	1262	1274	rBV2	12220	25748	1.50%	0.197%
7	10.957	1297	1305	1311	rBV	183915	346730	20.18%	2.651%
8	11.004	1311	1313	1319	rVB2	12375	18392	1.07%	0.141%
9	12.820	1616	1622	1628	rBV2	10435	17211	1.00%	0.132%
10	13.390	1712	1719	1730	rVB	855482	1333023	77.59%	10.192%
11	14.089	1831	1838	1843	rBV2	10864	20461	1.19%	0.156%
12	14.494	1901	1907	1913	rBV2	10956	21220	1.24%	0.162%
13	14.765	1943	1953	1960	rBV	297002	485784	28.27%	3.714%
14	14.829	1960	1964	1972	rVB	40675	64163	3.73%	0.491%
15	15.164	2015	2021	2027	rBV	25727	38655	2.25%	0.296%
16	15.810	2123	2131	2142	rVB	34896	60239	3.51%	0.461%
17	16.104	2177	2181	2187	rVB	13346	20750	1.21%	0.159%
18	16.257	2201	2207	2217	rBV	538289	893324	51.99%	6.830%
19	16.815	2290	2302	2307	rBV6	11367	35815	2.08%	0.274%
20	17.038	2332	2340	2344	rBV8	9997	22562	1.31%	0.173%
21	17.168	2356	2362	2369	rBV	23605	38467	2.24%	0.294%
22	17.238	2369	2374	2378	rBV4	14994	28134	1.64%	0.215%
23	17.338	2386	2391	2400	rVB	20853	35256	2.05%	0.270%
24	17.514	2413	2421	2425	rBV	354239	570416	33.20%	4.361%
25	17.561	2425	2429	2435	rVV	349981	525280	30.57%	4.016%
26	17.650	2437	2444	2449	rVV	80996	130252	7.58%	0.996%
27	17.920	2483	2490	2496	rBV2	29529	62256	3.62%	0.476%
28	18.096	2515	2520	2525	rVB4	9263	19814	1.15%	0.152%
29	18.390	2565	2570	2574	rBV	50766	79768	4.64%	0.610%
30	18.443	2574	2579	2585	rVB2	69860	120133	6.99%	0.919%
31	18.519	2587	2592	2597	rBV	31165	46939	2.73%	0.359%
32	18.584	2597	2603	2607	rBV2	64554	135140	7.87%	1.033%
33	18.883	2650	2654	2658	rBV	38967	55466	3.23%	0.424%
34	18.936	2658	2663	2670	rVB	30161	51064	2.97%	0.390%
35	19.124	2692	2695	2700	rVB2	16078	20852	1.21%	0.159%
36	19.301	2720	2725	2731	rBV2	28908	58609	3.41%	0.448%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.447	2746	2750	2756	rVB2	26273	45360	2.64%	0.347%
38	19.565	2765	2770	2776	rBV	497736	721656	42.00%	5.518%
39	19.665	2783	2787	2790	rBV2	17162	24677	1.44%	0.189%
40	19.894	2822	2826	2828	rBV2	76540	108231	6.30%	0.828%
41	19.929	2828	2832	2839	rVB	447967	635656	37.00%	4.860%
42	19.994	2840	2843	2849	rVB2	32442	45762	2.66%	0.350%
43	20.117	2858	2864	2869	rBV	1273645	1718122	100.00%	13.137%
44	21.192	3044	3047	3056	rVB	53113	83722	4.87%	0.640%
45	21.410	3081	3084	3090	rVB2	75219	128204	7.46%	0.980%
46	21.809	3144	3152	3157	rBV2	408180	1006257	58.57%	7.694%
47	21.856	3157	3160	3173	rVB	192370	332346	19.34%	2.541%
48	25.194	3721	3728	3737	rVB2	159086	450820	26.24%	3.447%

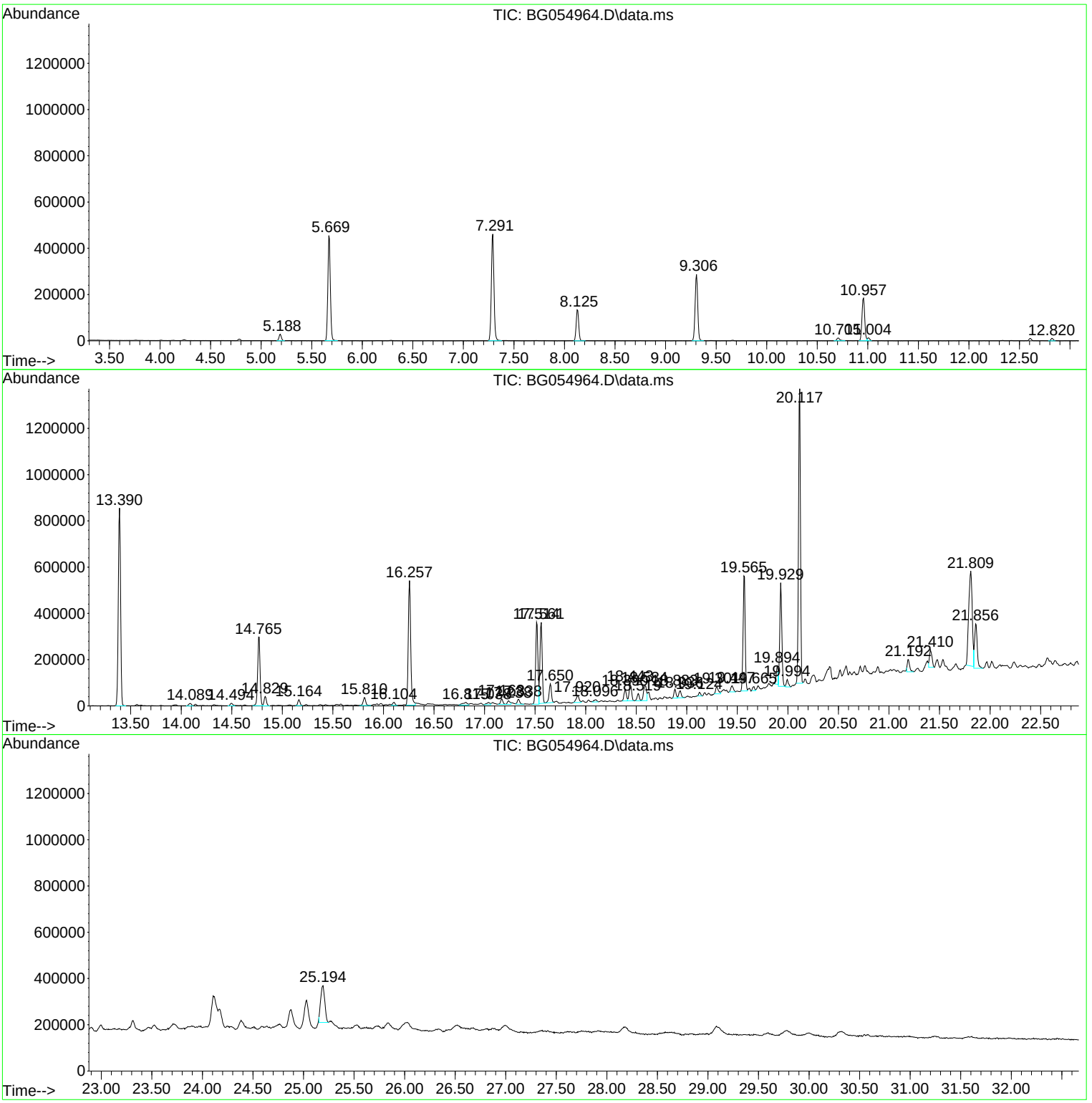
Sum of corrected areas: 13078517

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

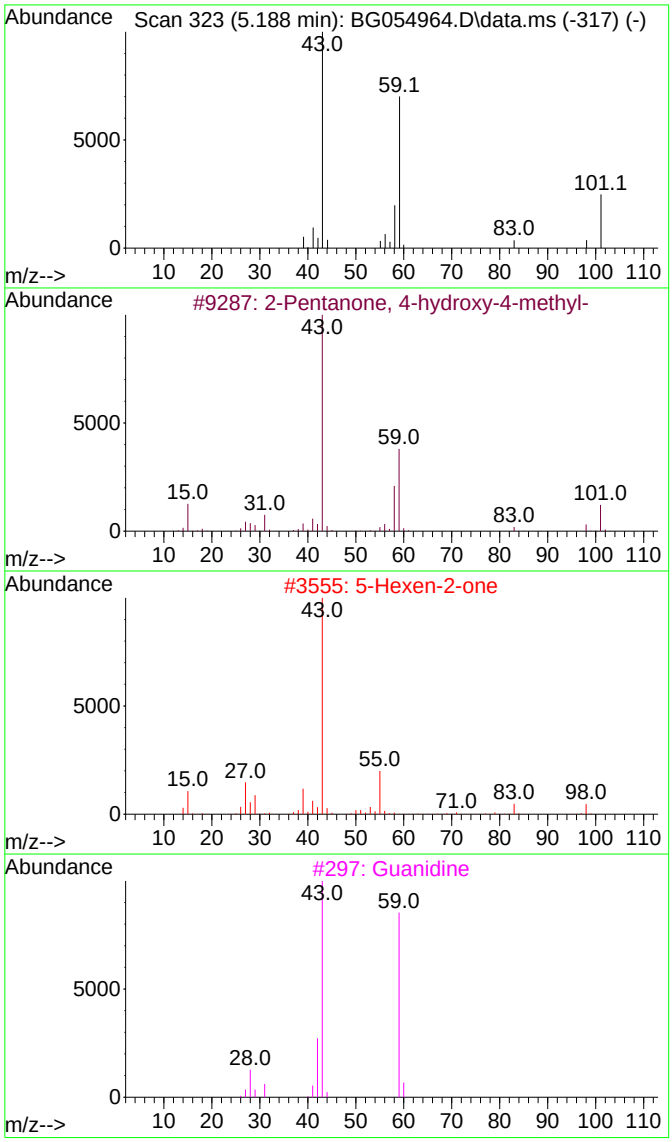
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

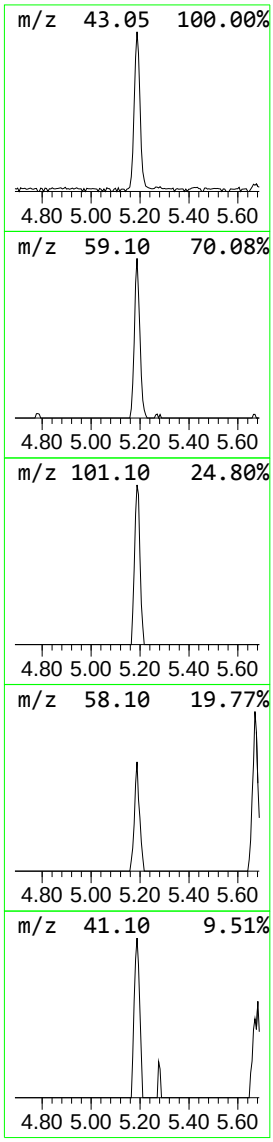
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.188	3.89 ng	45559	1,4-Dichlorobenzene-d4	8.125

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

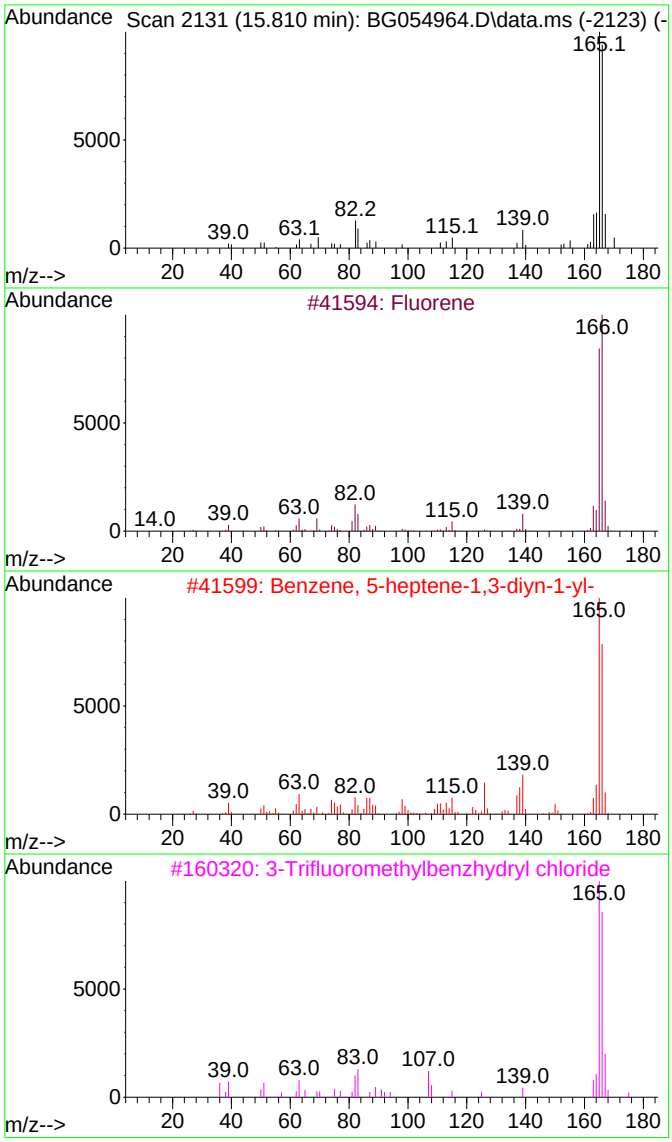
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

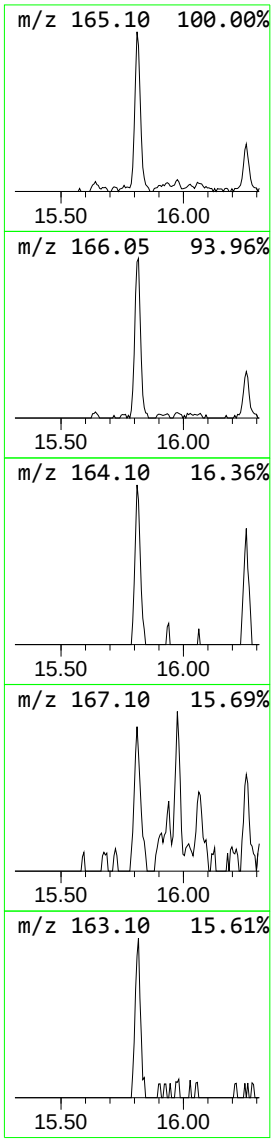
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 5-heptene-1,3-diyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.810	2.48 ng	60239	Acenaphthene-d10	14.771

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene	166	C13H10	000086-73-7	93
2	Benzene, 5-heptene-1,3-diyn-1-yl-	166	C13H10	013678-98-3	72
3	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	56
4	Benzaldehyde, 2,4-dihydroxy-3,6-...	166	C9H10O3	034883-14-2	50
5	1H-Phenalene	166	C13H10	000203-80-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

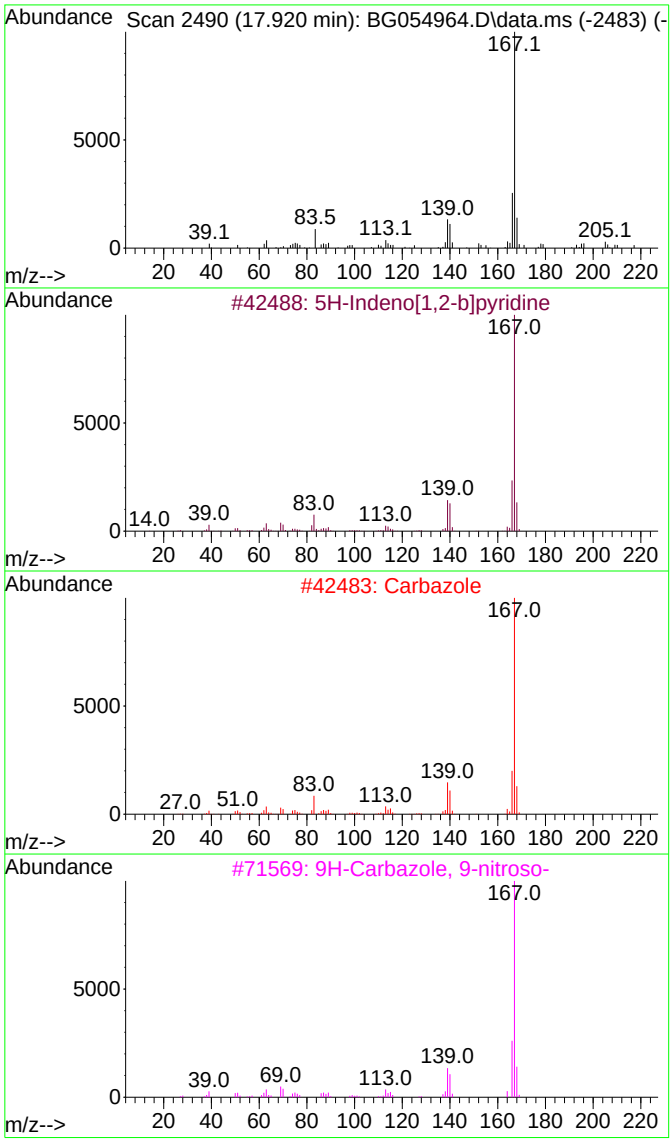
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

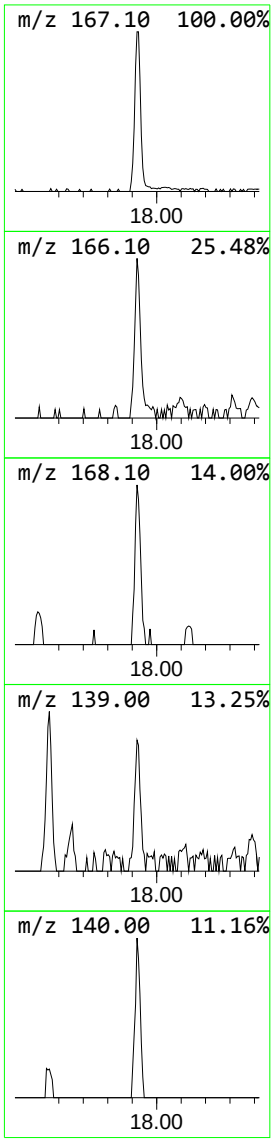
****

Peak Number 3 5H-Indeno[1,2-b]pyridine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.920	2.18 ng	62256	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	95
2	Carbazole	167	C12H9N	000086-74-8	95
3	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	91
4	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	90
5	ethanone, 1-(9H-carbazol-9-yl)-	209	C14H11NO	1000400-59-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

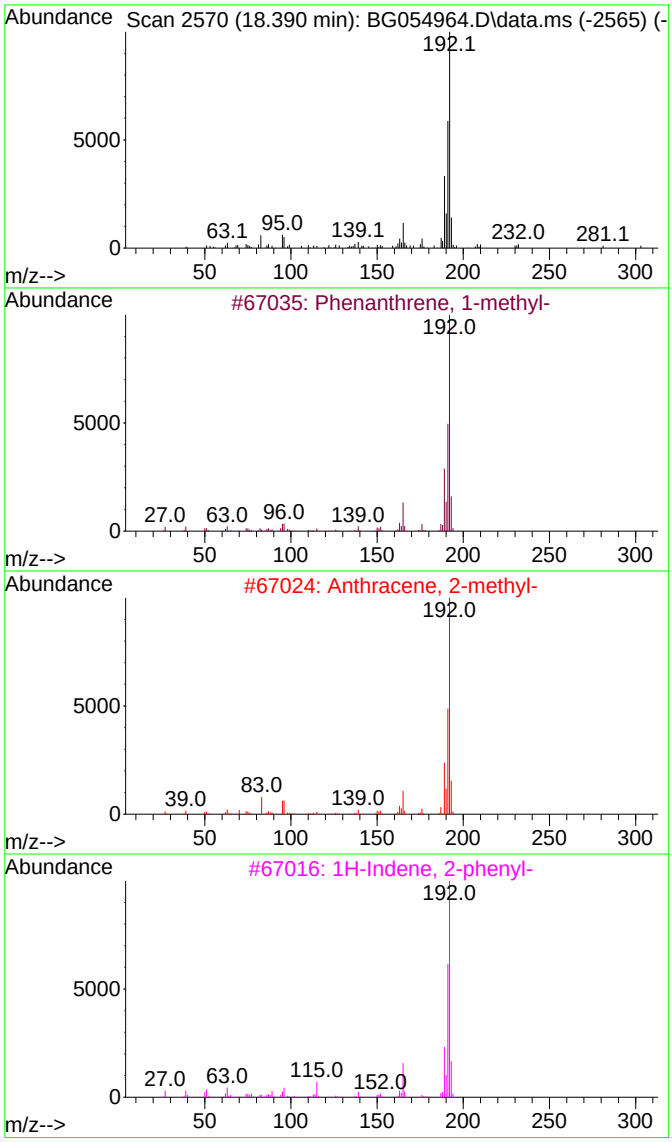
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

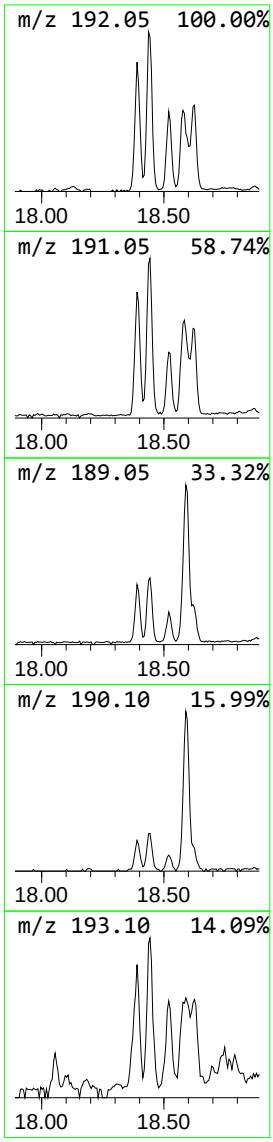
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	2.80 ng	79768	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

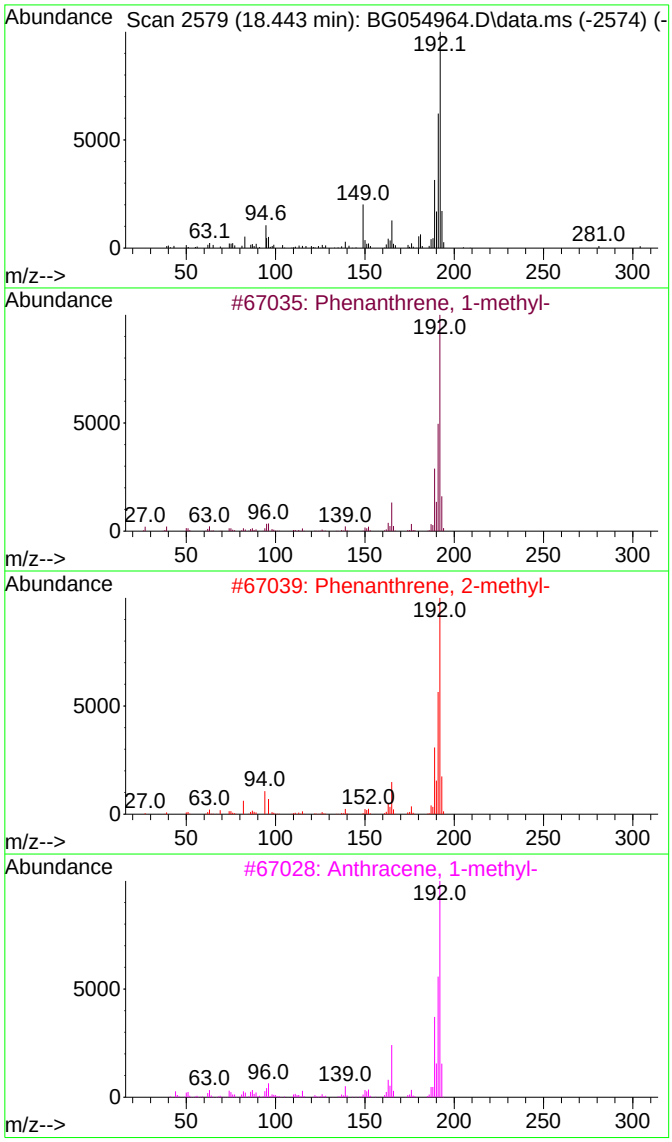
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

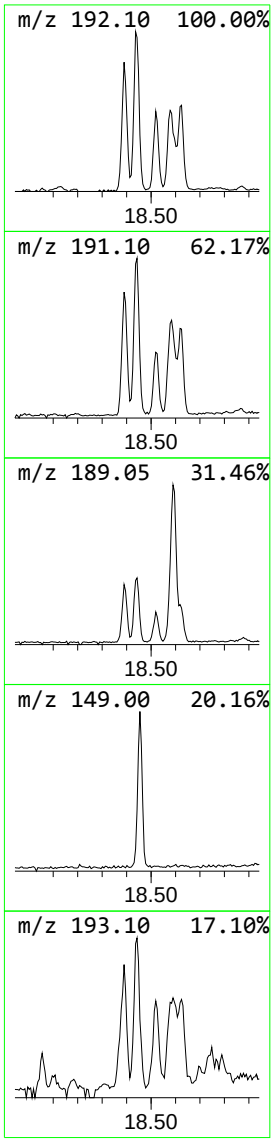
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.443	4.21 ng	120133	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

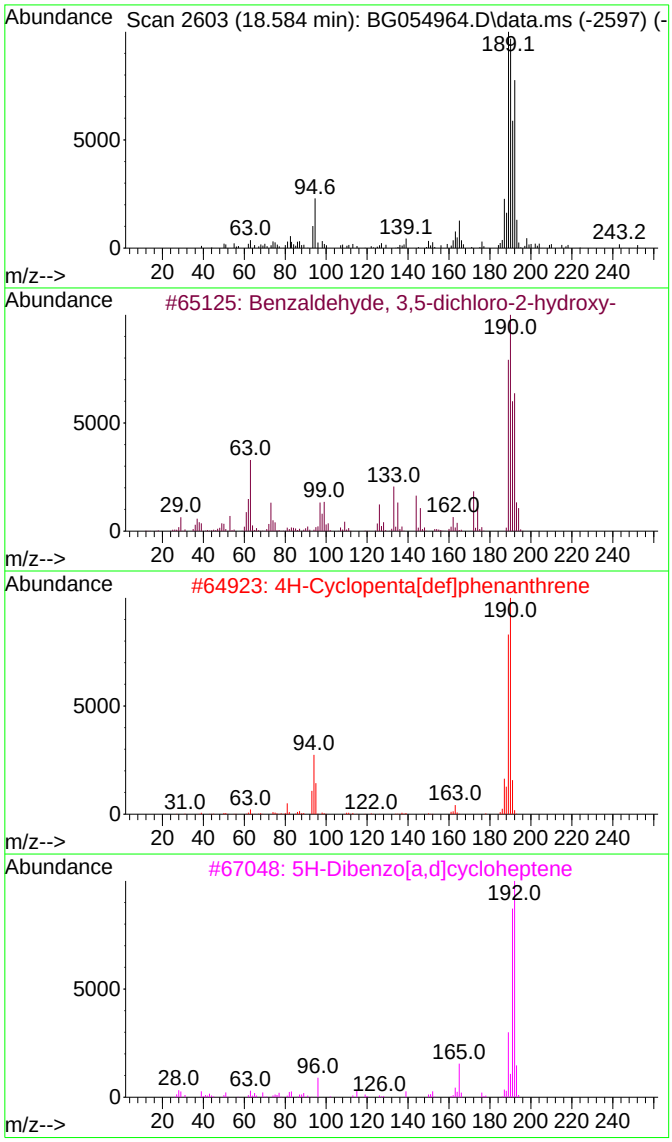
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

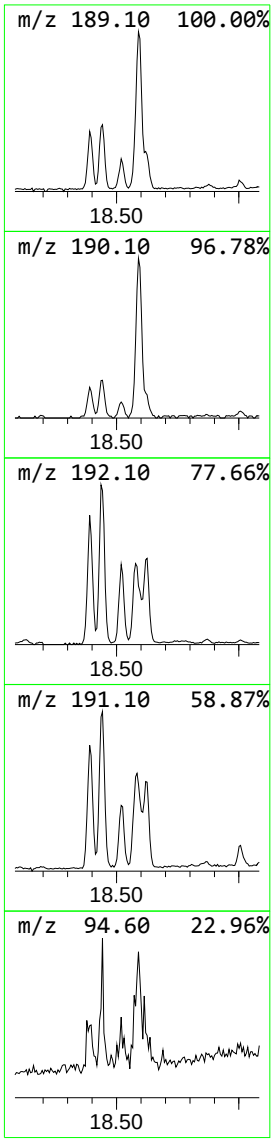
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.584	4.74 ng	135140	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	42
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

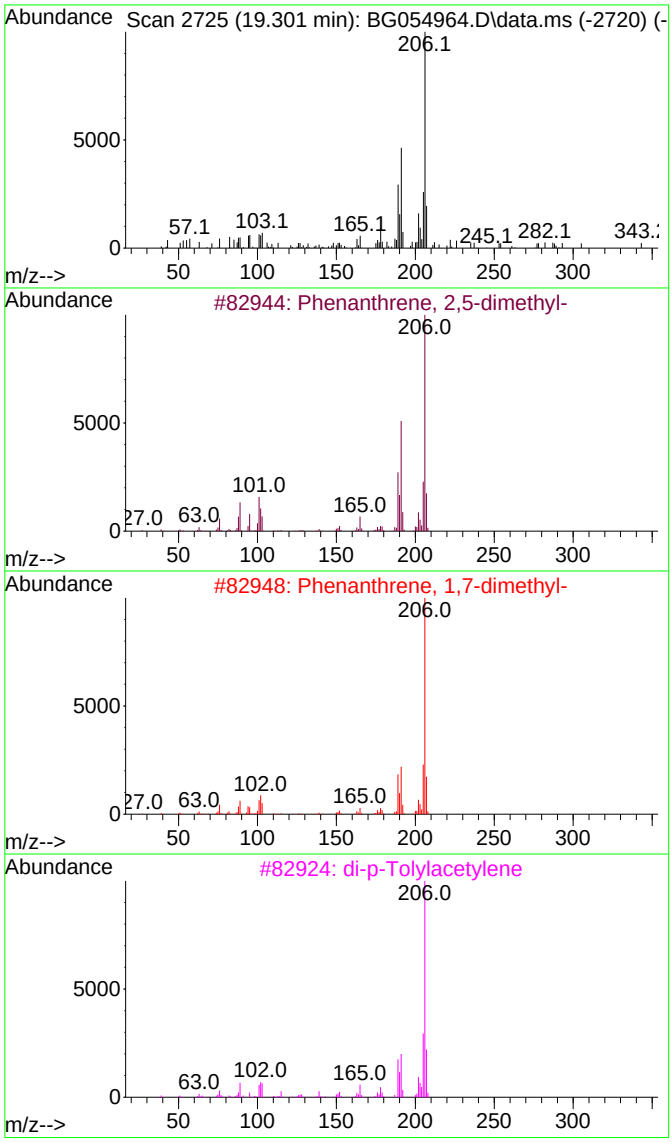
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

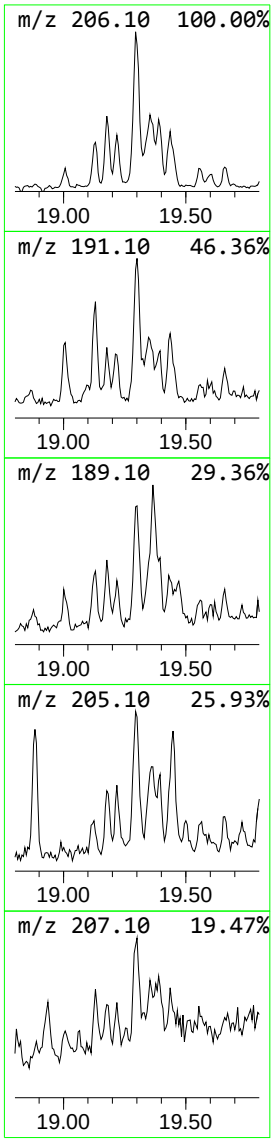
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.301	2.05 ng	58609	Phenanthrene-d10	17.514

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	92
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

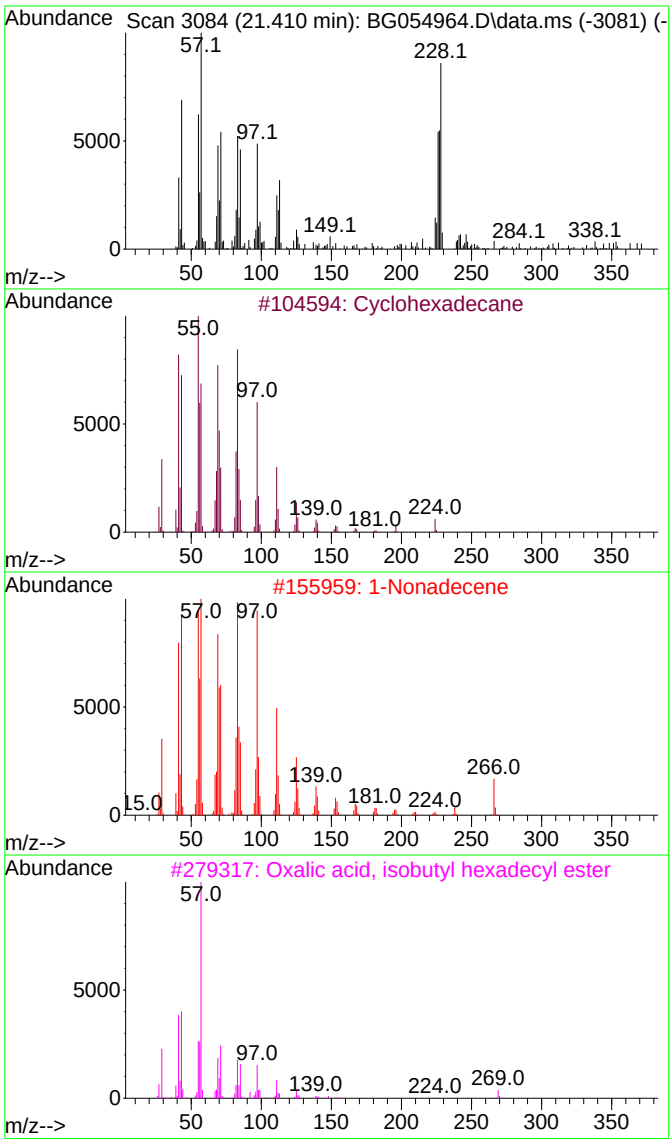
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

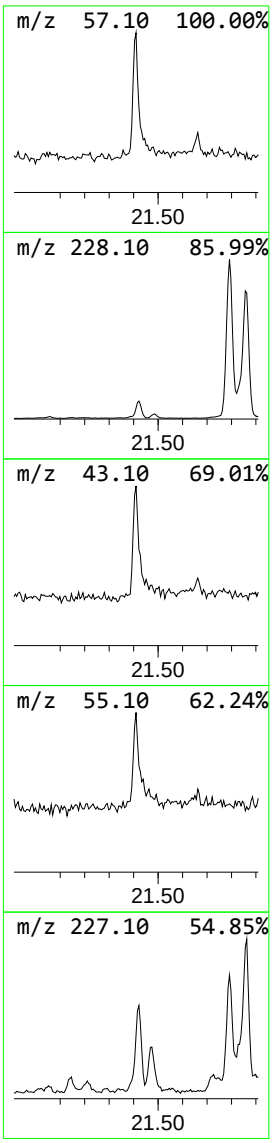
****

Peak Number 8 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	2.55 ng	128204	Chrysene-d12	21.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	56
2	1-Nonadecene	266	C19H38	018435-45-5	55
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	45
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	43
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054964.D
Acq On : 15 Sep 2022 20:21
Operator : CG/JU
Sample : N4569-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-6-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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-...	5.188	3.9	ng	45559	1	8.125	234097	20.0
Benzene, 5-hept...	15.810	2.5	ng	60239	3	14.771	485784	20.0
5H-Indeno[1,2-b...	17.920	2.2	ng	62256	4	17.514	570416	20.0
Phenanthrene, 1...	18.390	2.8	ng	79768	4	17.514	570416	20.0
Phenanthrene, 2...	18.443	4.2	ng	120133	4	17.514	570416	20.0
Benzaldehyde, 3...	18.584	4.7	ng	135140	4	17.514	570416	20.0
Phenanthrene, 2...	19.301	2.0	ng	58609	4	17.514	570416	20.0
Cyclohexadecane	21.410	2.5	ng	128204	5	21.809	1006260	20.0