LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057782.D
Acq On : 20 Jun 2023 19:01
Operator : CG/JU
Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	19	rVB	61004	116422	13.04%	1.198%
2	5.039	326	332	340	rBV	55372	87088	9.76%	0.896%
3	5.503	404	411	420	rBV	252844	409616	45.88%	4.215%
4	7.089	673	681	689	rBV	324333	548761	61.47%	5.647%
5	7.930	816	824	837	rVB	191008	329431	36.90%	3.390%
6	8.065	840	847	853	rVB4	6367	11947	1.34%	0.123%
7	8.687	948	953	959	rBV3	5085	9787	1.10%	0.101%
8	9.087	1014	1021	1030	rBV	191844	334997	37.52%	3.447%
9	10.368	1233	1239	1244	rVB2	13052	21664	2.43%	0.223%
10	10.732	1290	1301	1307	rBV	270548	472735	52.95%	4.865%
11	10.785	1307	1310	1317	rVB2	16408	23976	2.69%	0.247%
12	12.148	1536	1542	1547	rBV4	5141	10097	1.13%	0.104%
13	12.389	1577	1583	1588	rVB2	13008	20025	2.24%	0.206%
14	12.606	1614	1620	1628	rVB2	7971	14819	1.66%	0.153%
15	13.188	1712	1719	1727	rVB	465764	730379	81.81%	7.516%
16	13.376	1740	1751	1752	rBV3	10703	19611	2.20%	0.202%
17	13.887	1832	1838	1842	rBV4	9871	17834	2.00%	0.184%
18	13.940	1842	1847	1852	rVV2	6285	9947	1.11%	0.102%
19	14.293	1901	1907	1912	rBV2	8365	16016	1.79%	0.165%
20	14.463	1931	1936	1941	rBV4	10790	18464	2.07%	0.190%
21	14.563	1943	1953	1959	rBV	389934	591528	66.26%	6.087%
22	14.628	1959	1964	1967	rBV2	19410	27990	3.14%	0.288%
23	14.739	1977	1983	1991	rBV	32581	57229	6.41%	0.589%
24	14.957	2015	2020	2026	rBV2	19750	30179	3.38%	0.311%
25	15.027	2026	2032	2037	rVB6	7527	14197	1.59%	0.146%
26	15.127	2043	2049	2055	rBV2	15356	30308	3.39%	0.312%
27	15.603	2125	2130	2140	rBV2	21063	40461	4.53%	0.416%
28	15.732	2145	2152	2156	rBV6	6381	12486	1.40%	0.128%
29	15.914	2176	2183	2189	rVB3	28873	50992	5.71%	0.525%
30	16.044	2199	2205	2214	rBV	111982	178562	20.00%	1.838%
31	16.120	2214	2218	2226	rVV8	6374	12935	1.45%	0.133%
32	16.273	2239	2244	2245	rBV3	13080	16646	1.86%	0.171%
33	16.760	2324	2327	2332	rVB6	13950	15834	1.77%	0.163%
34	16.960	2356	2361	2368	rVB4	12489	20876	2.34%	0.215%
35	17.066	2376	2379	2382	rVB3	9153	10408	1.17%	0.107%
36	17.125	2385	2389	2393	rBV2	13166	19393	2.17%	0.200%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057782.D
Acq On : 20 Jun 2023 19:01
Operator : CG/JU
Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.307	2414	2420	2424	rBV	450357	671107	75.17%	6.906%
38	17.348	2424	2427	2432	rVB	176743	243357	27.26%	2.504%
39	17.442	2438	2443	2446	rBV	40025	55265	6.19%	0.569%
40	17.706	2485	2488	2493	rVB2	15581	20066	2.25%	0.207%
41	18.194	2565	2571	2574	rBV3	81247	125887	14.10%	1.296%
42	18.229	2574	2577	2582	rVB	37893	56551	6.33%	0.582%
43	18.376	2597	2602	2606	rBV3	50417	92466	10.36%	0.952%
44	18.494	2619	2622	2626	rBV3	13128	19004	2.13%	0.196%
45	18.529	2626	2628	2630	rVV3	13543	13008	1.46%	0.134%
46	18.570	2631	2635	2645	rVB	105139	173003	19.38%	1.780%
47	18.682	2652	2654	2657	rVB	19055	16438	1.84%	0.169%
48	18.881	2683	2688	2693	rBV	84911	128962	14.45%	1.327%
49	18.928	2693	2696	2699	rVB4	20629	26195	2.93%	0.270%
50	19.058	2714	2718	2722	rBV3	51838	75567	8.46%	0.778%
51	19.363	2764	2770	2774	rBV	383181	552076	61.84%	5.681%
52	19.416	2774	2779	2784	rVB	531459	660153	73.95%	6.794%
53	19.722	2822	2831	2839	rBV	321749	586720	65.72%	6.038%
54	19.921	2860	2865	2870	rBV	680000	840573	94.16%	8.650%
55	21.455	3123	3126	3131	rVB2	95122	114393	12.81%	1.177%
56	21.561	3137	3144	3149	rBV2	412636	892746	100.00%	9.187%

Sum of corrected areas: 9717177

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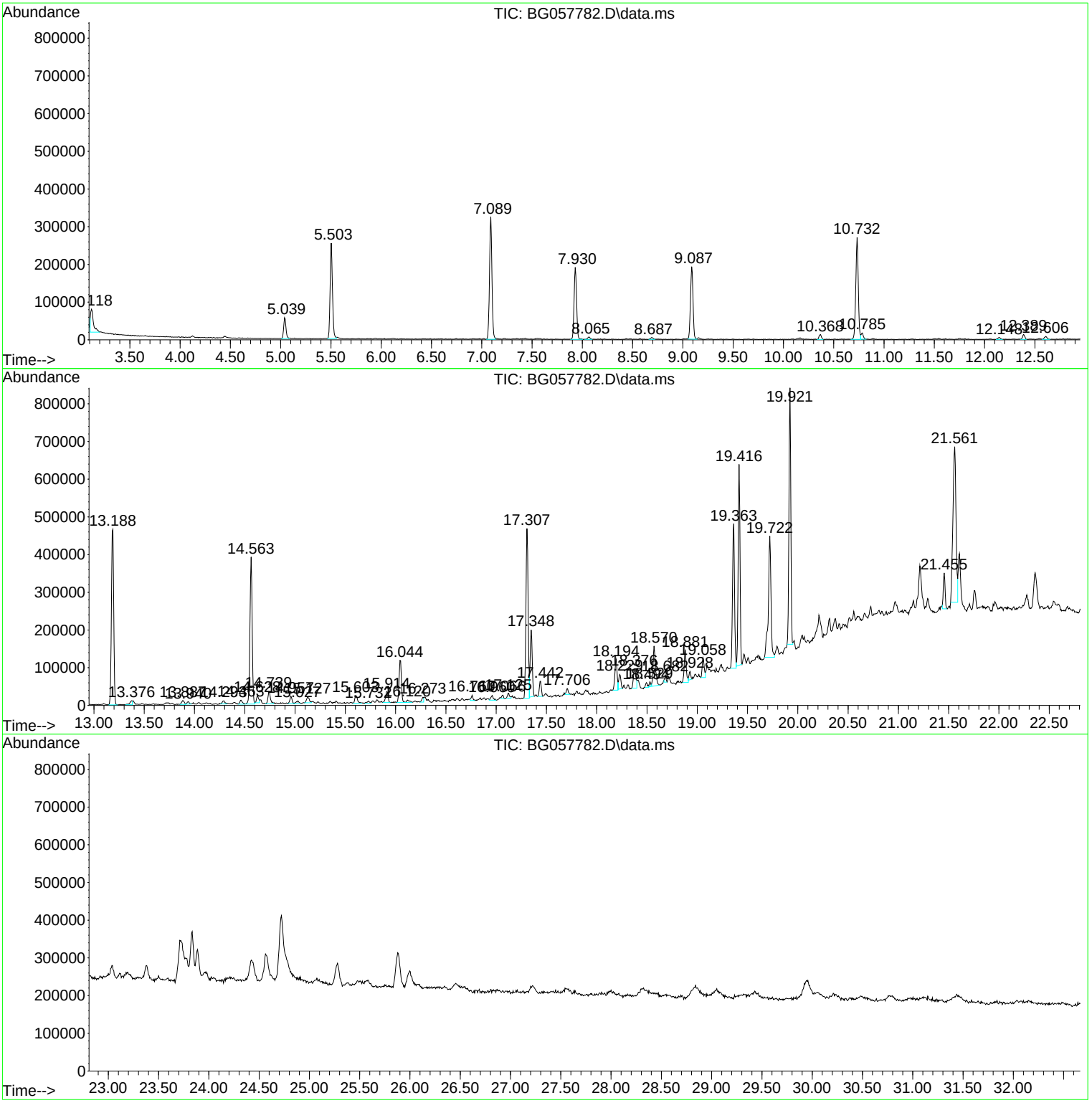
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057782.D
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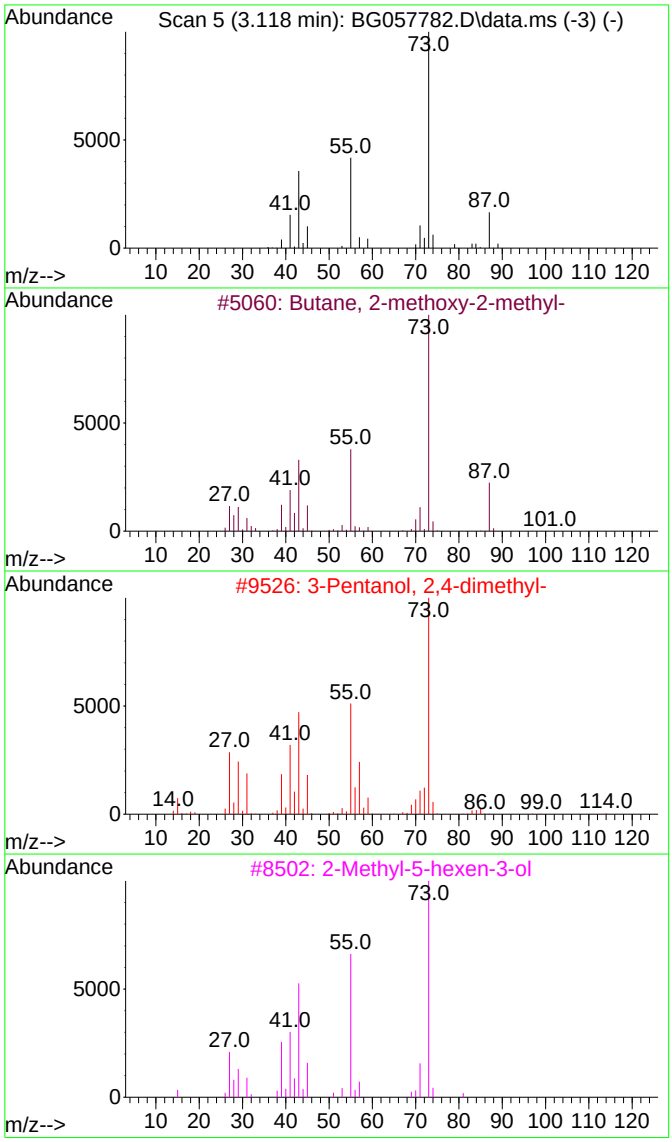
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

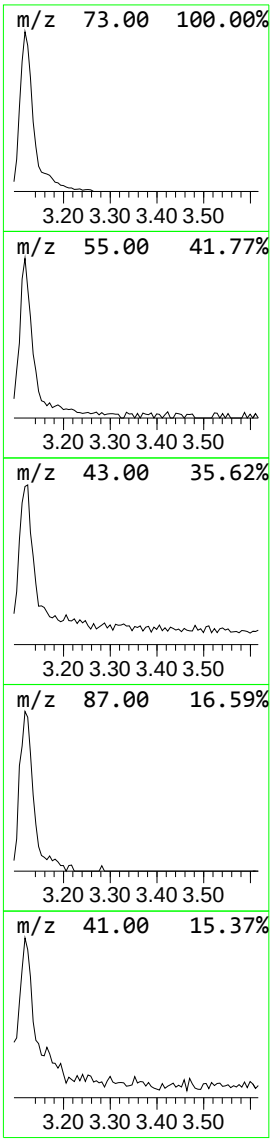
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	7.07 ng	116422	1,4-Dichlorobenzene-d4	7.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	36
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057782.D
Acq On : 20 Jun 2023 19:01
Operator : CG/JU
Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

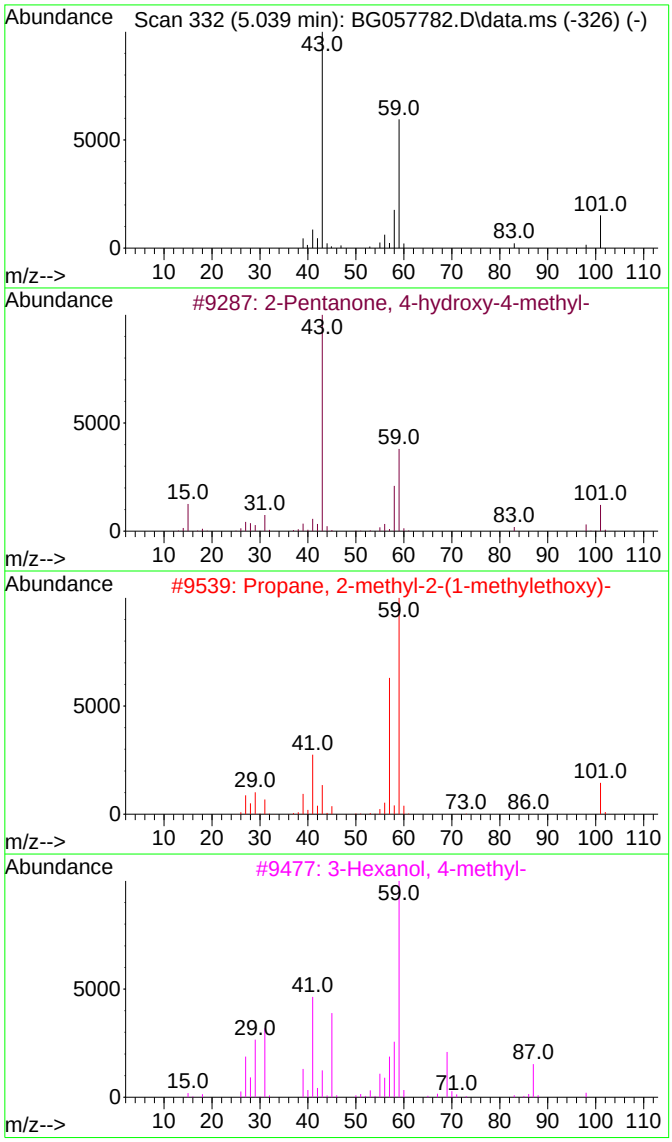
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

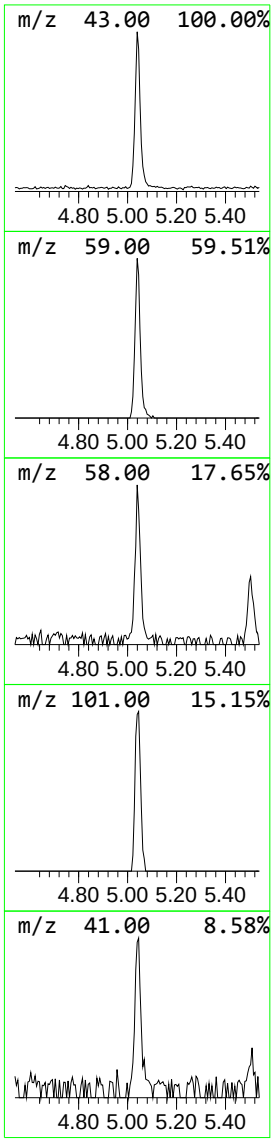
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	5.29 ng	87088	1,4-Dichlorobenzene-d4	7.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
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Acq On : 20 Jun 2023 19:01
Operator : CG/JU
Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

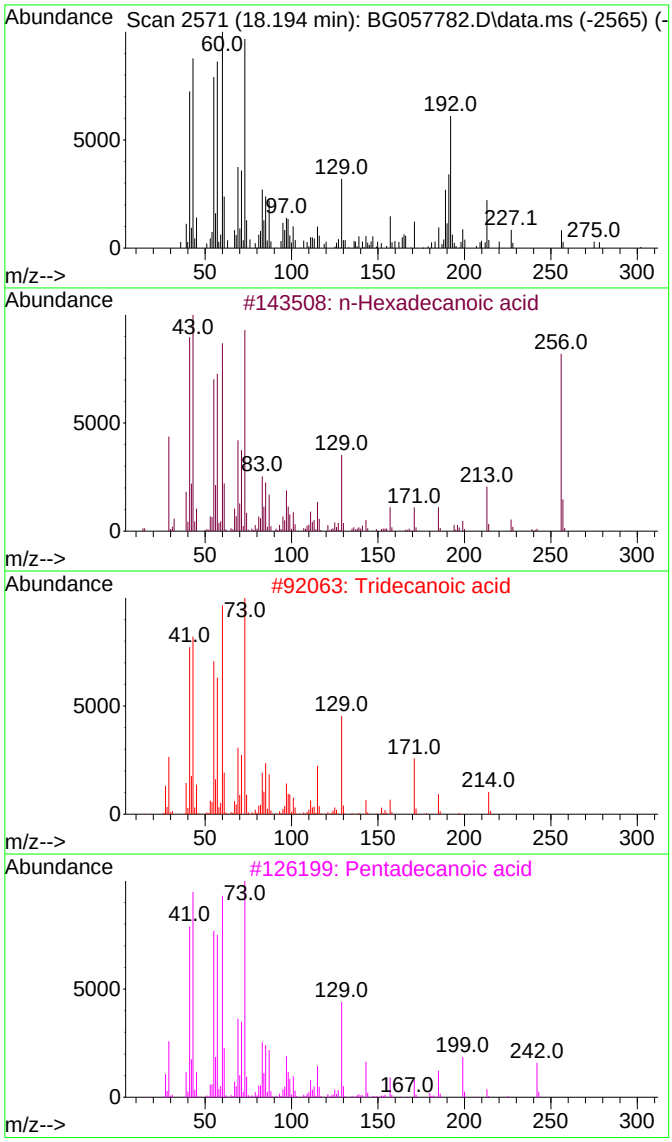
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

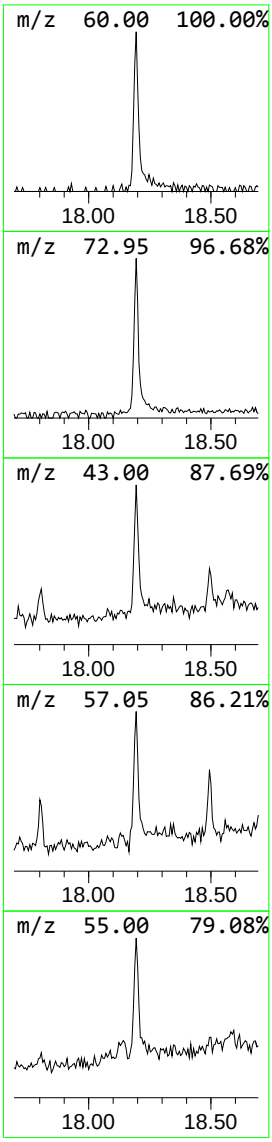
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.194	3.75 ng	125887	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	55
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
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Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

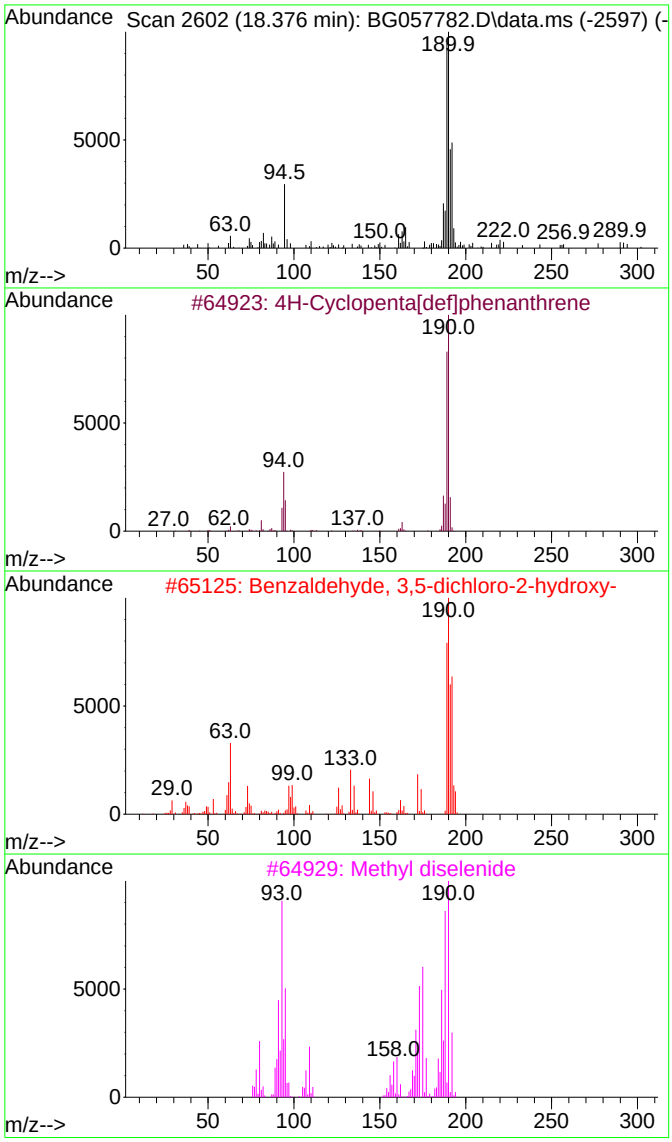
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

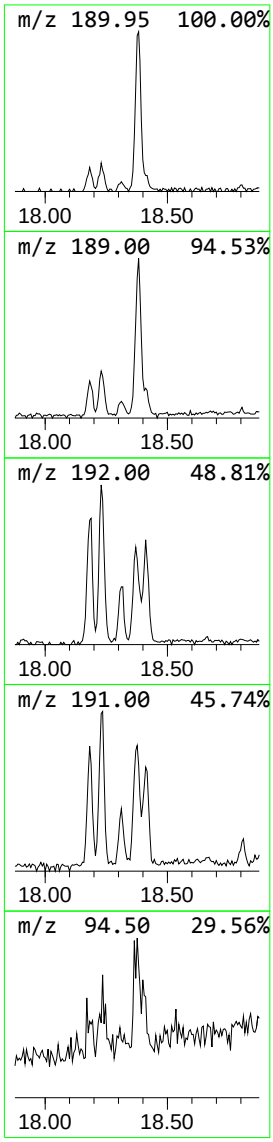
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.376	2.76 ng	92466	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
5	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

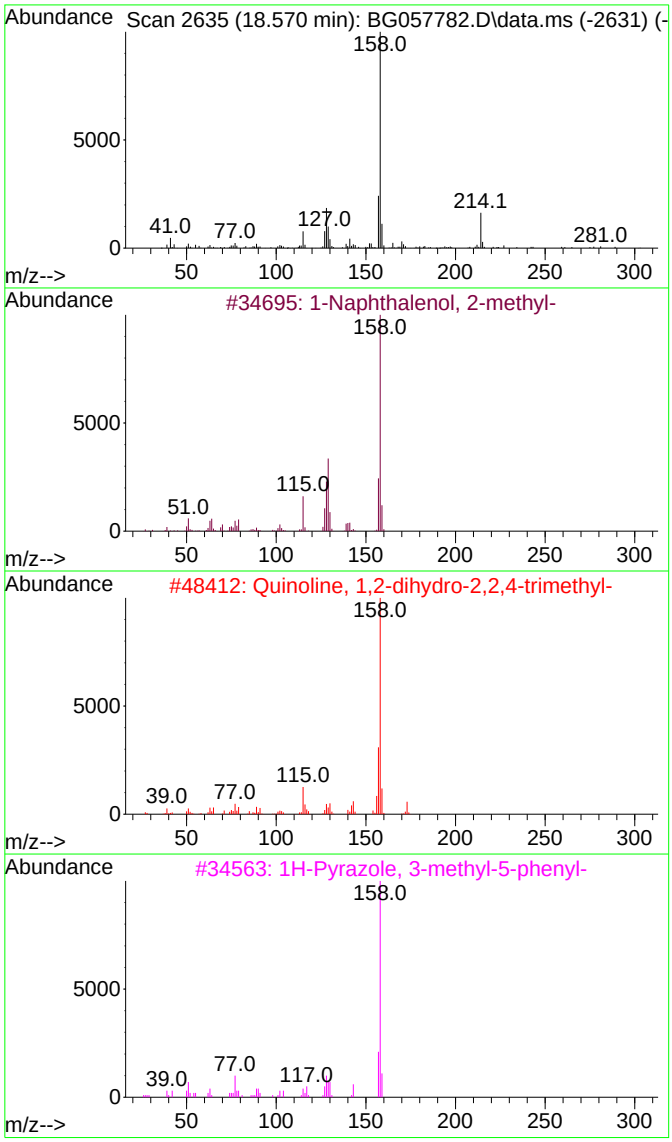
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

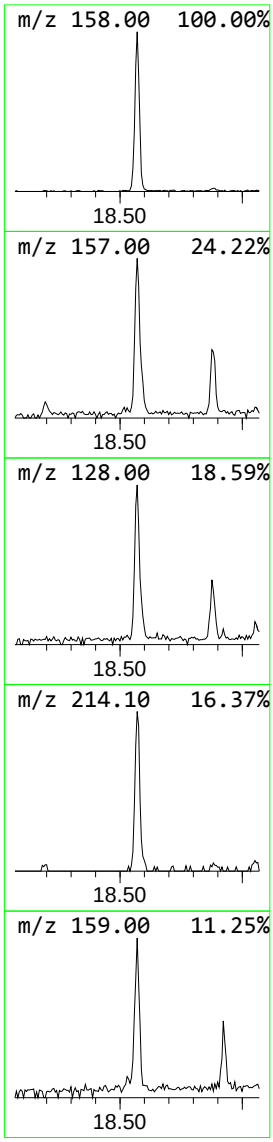
****

Peak Number 5 1-Naphthalenol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.570	5.16 ng	173003	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, 2-methyl-	158	C11H10O	007469-77-4	72
2	Quinoline, 1,2-dihydro-2,2,4-tri...	173	C12H15N	000147-47-7	64
3	1H-Pyrazole, 3-methyl-5-phenyl-	158	C10H10N2	003347-62-4	64
4	6-Quinolinamine, 2-methyl-	158	C10H10N2	065079-19-8	59
5	8-Hydroxy-5-(hydroxymethyl)quino...	315	C18H21NO4	1000463-60-9	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

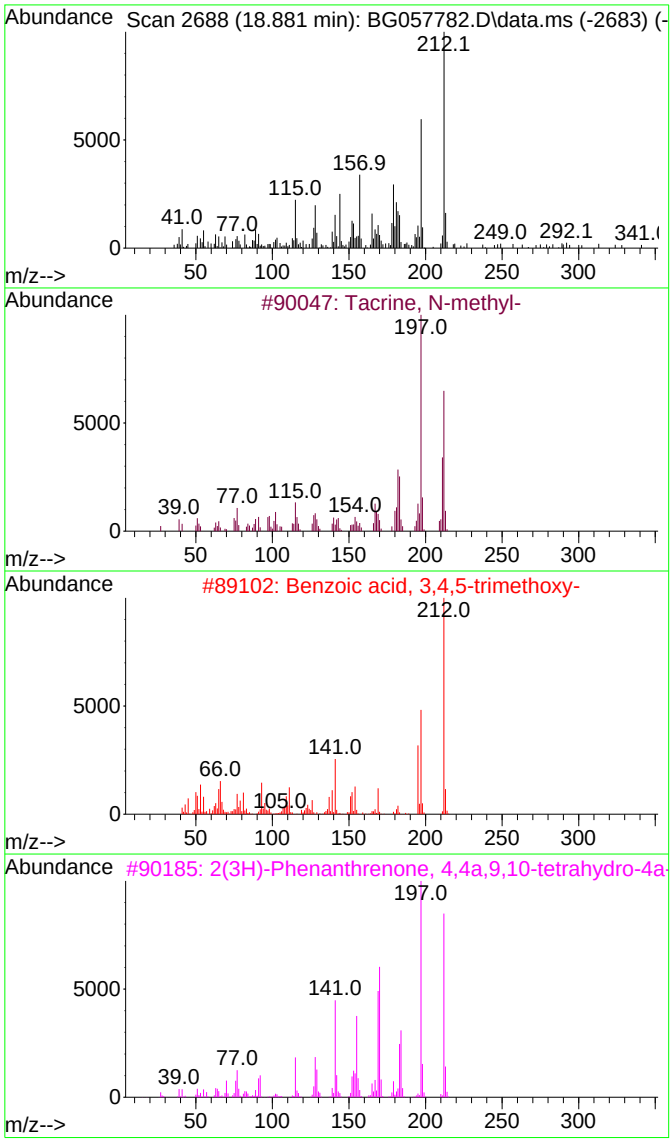
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

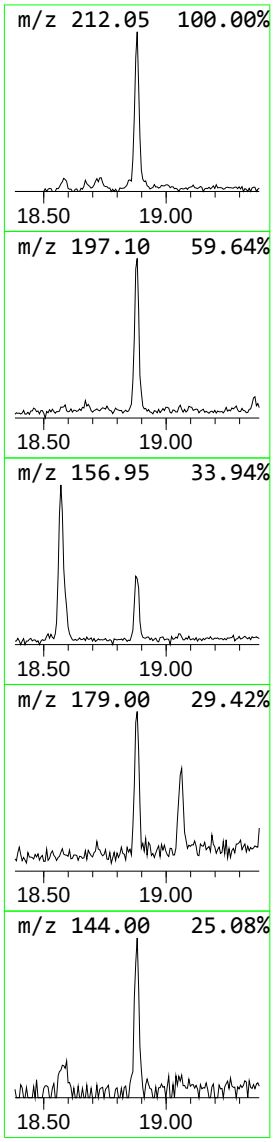
****

Peak Number 6 Tacrine, N-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.881	3.84 ng	128962	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tacrine, N-methyl-	212	C14H16N2	1000452-04-1	78
2	Benzoic acid, 3,4,5-trimethoxy-	212	C10H12O5	000118-41-2	60
3	2(3H)-Phenanthrenone, 4,4a,9,10-...	212	C15H16O	006606-34-4	53
4	2,5-Dimethyl-4-(3-amino-4-methyl...	212	C14H16N2	071153-33-8	53
5	2,3-Dimethoxy-5-methylhydroquino...	212	C11H16O4	035896-58-3	49





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

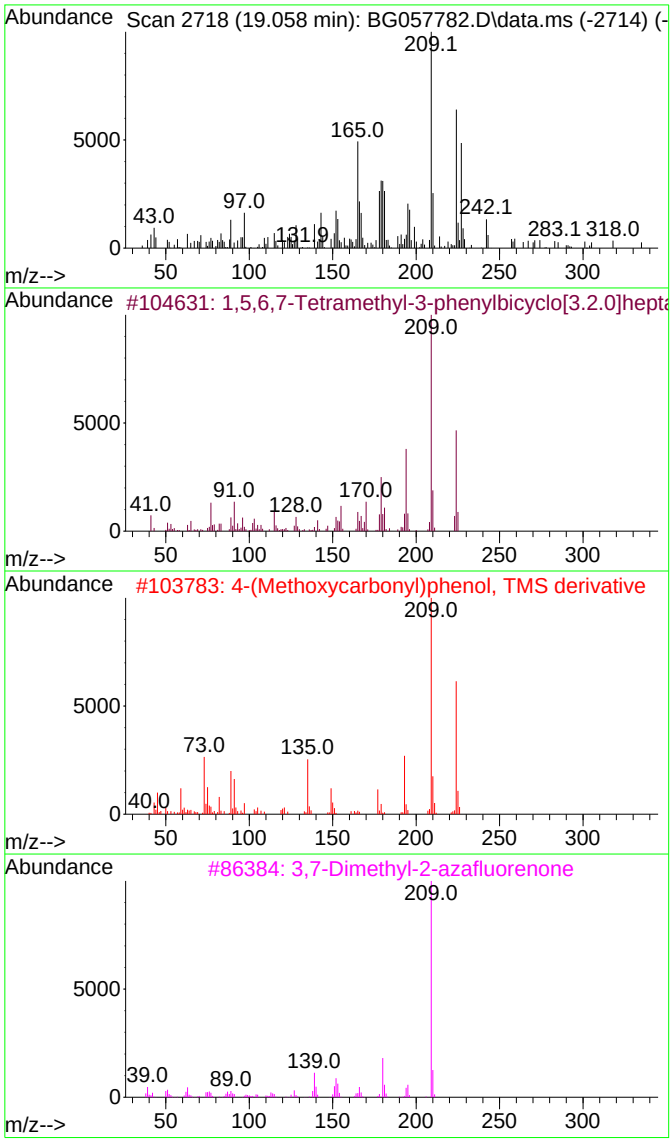
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

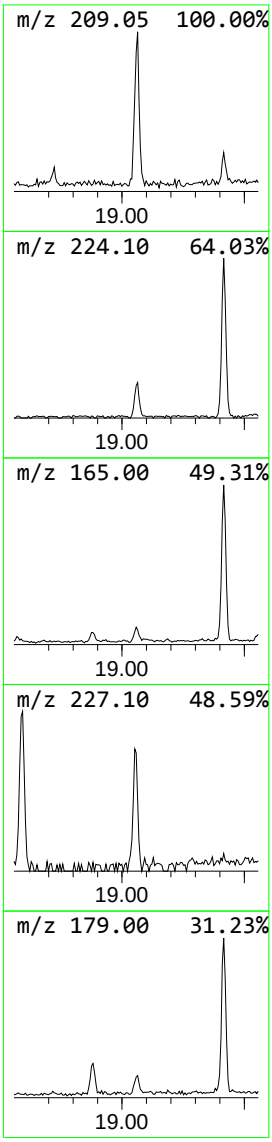
****

Peak Number 7 unknown19.058 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.058	2.25 ng	75567	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,6,7-Tetramethyl-3-phenylbicy...	224	C17H20	126584-00-7	46
2	4-(Methoxycarbonyl)phenol, TMS d...	224	C11H16O3Si	027739-17-9	38
3	3,7-Dimethyl-2-azafluorenone	209	C14H11NO	019337-28-1	38
4	Silane, dimethyl(3-ethylphenoxy)...	224	C12H20O2Si	1000347-46-1	38
5	Dimethylbis(thiophen-2-yl)silane	224	C10H12S2Si	1000487-00-9	35





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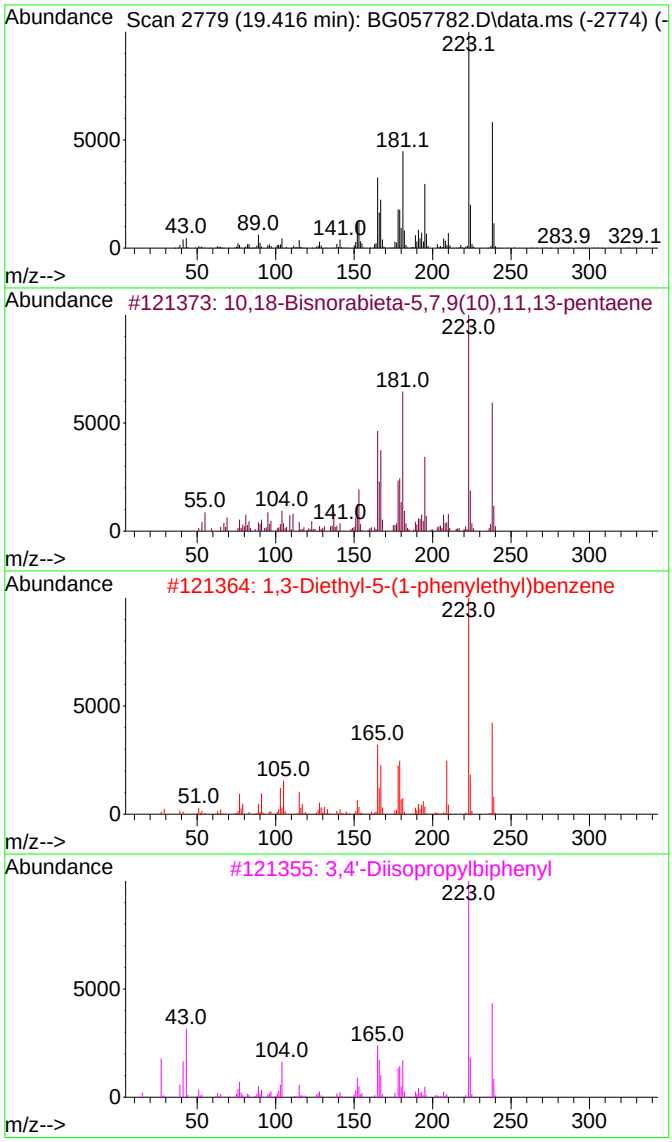
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

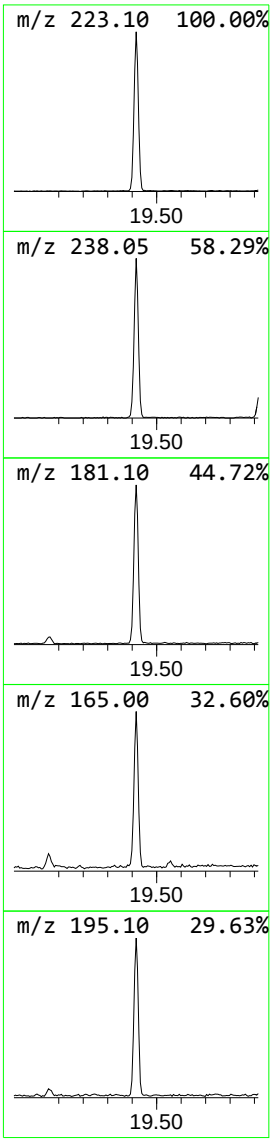
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	19.67 ng	660153	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89
3	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	89
4	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	64
5	4,4'-Diacetyl biphenyl	238	C16H14O2	000787-69-9	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057782.D
Acq On : 20 Jun 2023 19:01
Operator : CG/JU
Sample : 03255-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSIT-SB-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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
Butane, 2-metho...	3.118	7.1	ng	116422	1	7.930	329431	20.0
2-Pentanone, 4-...	5.039	5.3	ng	87088	1	7.930	329431	20.0
n-Hexadecanoic ...	18.194	3.8	ng	125887	4	17.307	671107	20.0
4H-Cyclopenta[d...	18.376	2.8	ng	92466	4	17.307	671107	20.0
1-Naphthalenol,...	18.570	5.2	ng	173003	4	17.307	671107	20.0
Tacrine, N-methyl-	18.881	3.8	ng	128962	4	17.307	671107	20.0
unknown19.058	19.058	2.3	ng	75567	4	17.307	671107	20.0
10,18-Bisnorabi...	19.416	19.7	ng	660153	4	17.307	671107	20.0