LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064159.D
Acq On : 2 Apr 2025 19:04
Operator : RC/JU
Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

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: BG064159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	317	323	331	rBV	95843	150100	13.47%	1.402%
2	5.451	395	402	412	rVB	373725	621755	55.78%	5.806%
3	6.056	500	505	511	rVB2	14974	24353	2.18%	0.227%
4	7.025	662	670	681	rBV	403461	668933	60.01%	6.246%
5	7.860	805	812	820	rVB	178919	295398	26.50%	2.758%
6	9.011	1000	1008	1016	rVB	242154	423974	38.04%	3.959%
7	10.651	1278	1287	1294	rBV	235378	426660	38.28%	3.984%
8	10.821	1312	1316	1321	rVB4	7452	12955	1.16%	0.121%
9	11.691	1458	1464	1468	rBV4	10850	17414	1.56%	0.163%
10	12.078	1525	1530	1537	rBV6	5769	11229	1.01%	0.105%
11	12.296	1565	1567	1577	rVB6	6438	11294	1.01%	0.105%
12	13.036	1688	1693	1698	rBV4	19703	28141	2.52%	0.263%
13	13.107	1698	1705	1712	rVV	573628	870131	78.06%	8.125%
14	13.853	1828	1832	1837	rBV7	7684	11526	1.03%	0.108%
15	13.982	1851	1854	1858	rVB3	17646	24784	2.22%	0.231%
16	14.393	1921	1924	1929	rBV4	16399	20600	1.85%	0.192%
17	14.481	1929	1939	1947	rBV	366332	581834	52.20%	5.433%
18	14.887	2006	2008	2015	rVB7	8941	16652	1.49%	0.155%
19	14.951	2018	2019	2026	rVV5	9133	12099	1.09%	0.113%
20	15.016	2026	2030	2038	rVB7	11026	22290	2.00%	0.208%
21	15.269	2067	2073	2079	rBV10	4605	12568	1.13%	0.117%
22	15.345	2082	2086	2091	rVB3	20906	28561	2.56%	0.267%
23	15.533	2112	2118	2120	rBV6	8972	15316	1.37%	0.143%
24	15.750	2150	2155	2159	rBV5	15412	27414	2.46%	0.256%
25	15.839	2164	2170	2177	rVB	155604	215835	19.36%	2.015%
26	15.968	2185	2192	2200	rBV	511363	755665	67.79%	7.056%
27	16.209	2229	2233	2235	rBV3	27726	35693	3.20%	0.333%
28	16.403	2262	2266	2273	rVB2	28829	41457	3.72%	0.387%
29	16.585	2293	2297	2301	rBV7	6848	11646	1.04%	0.109%
30	17.002	2364	2368	2371	rBV2	23905	28576	2.56%	0.267%
31	17.049	2371	2376	2380	rVB5	18206	32225	2.89%	0.301%
32	17.225	2400	2406	2410	rBV2	423104	665123	59.67%	6.211%
33	17.266	2410	2413	2418	rVV	79874	107477	9.64%	1.004%
34	17.349	2425	2427	2434	rVB3	17659	24060	2.16%	0.225%
35	17.613	2468	2472	2478	rBV3	56760	82516	7.40%	0.771%
36	17.736	2488	2493	2499	rBV4	34085	43245	3.88%	0.404%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064159.D
Acq On : 2 Apr 2025 19:04
Operator : RC/JU
Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

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	18.124	2550	2559	2567	rBV4	145438	292941	26.28%	2.735%
38	18.224	2574	2576	2581	rVB6	11425	13284	1.19%	0.124%
39	18.289	2582	2587	2591	rVV4	41966	77845	6.98%	0.727%
40	18.324	2591	2593	2597	rVB4	19453	26687	2.39%	0.249%
41	18.424	2606	2610	2614	rBV2	38302	53521	4.80%	0.500%
42	18.494	2619	2622	2626	rVB4	14866	17283	1.55%	0.161%
43	18.553	2629	2632	2636	rBV2	53853	72513	6.51%	0.677%
44	18.594	2636	2639	2642	rBV5	15867	23843	2.14%	0.223%
45	18.817	2674	2677	2680	rBV4	13779	19496	1.75%	0.182%
46	18.894	2687	2690	2693	rBV5	14004	17313	1.55%	0.162%
47	19.011	2707	2710	2714	rBV3	25782	41387	3.71%	0.386%
48	19.058	2714	2718	2724	rVB5	59150	110668	9.93%	1.033%
49	19.276	2750	2755	2761	rBV	206359	303884	27.26%	2.838%
50	19.399	2773	2776	2780	rBV6	37240	54072	4.85%	0.505%
51	19.517	2792	2796	2799	rBV6	28622	46440	4.17%	0.434%
52	19.605	2809	2811	2812	rBV	22303	19209	1.72%	0.179%
53	19.634	2812	2816	2826	rVB	242823	356189	31.95%	3.326%
54	19.722	2827	2831	2835	rVB6	26383	42900	3.85%	0.401%
55	19.840	2846	2851	2856	rBV	898611	1114692	100.00%	10.409%
56	20.169	2903	2907	2910	rBV	56815	63189	5.67%	0.590%
57	20.657	2988	2990	2994	rVB2	55465	61852	5.55%	0.578%
58	21.138	3068	3072	3077	rVB5	101163	162505	14.58%	1.517%
59	21.450	3119	3125	3130	rBV3	464443	837802	75.16%	7.823%
60	24.470	3633	3639	3646	rBV2	221024	500009	44.86%	4.669%

Sum of corrected areas: 10709023

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ALS Vial : 14 Sample Multiplier: 1

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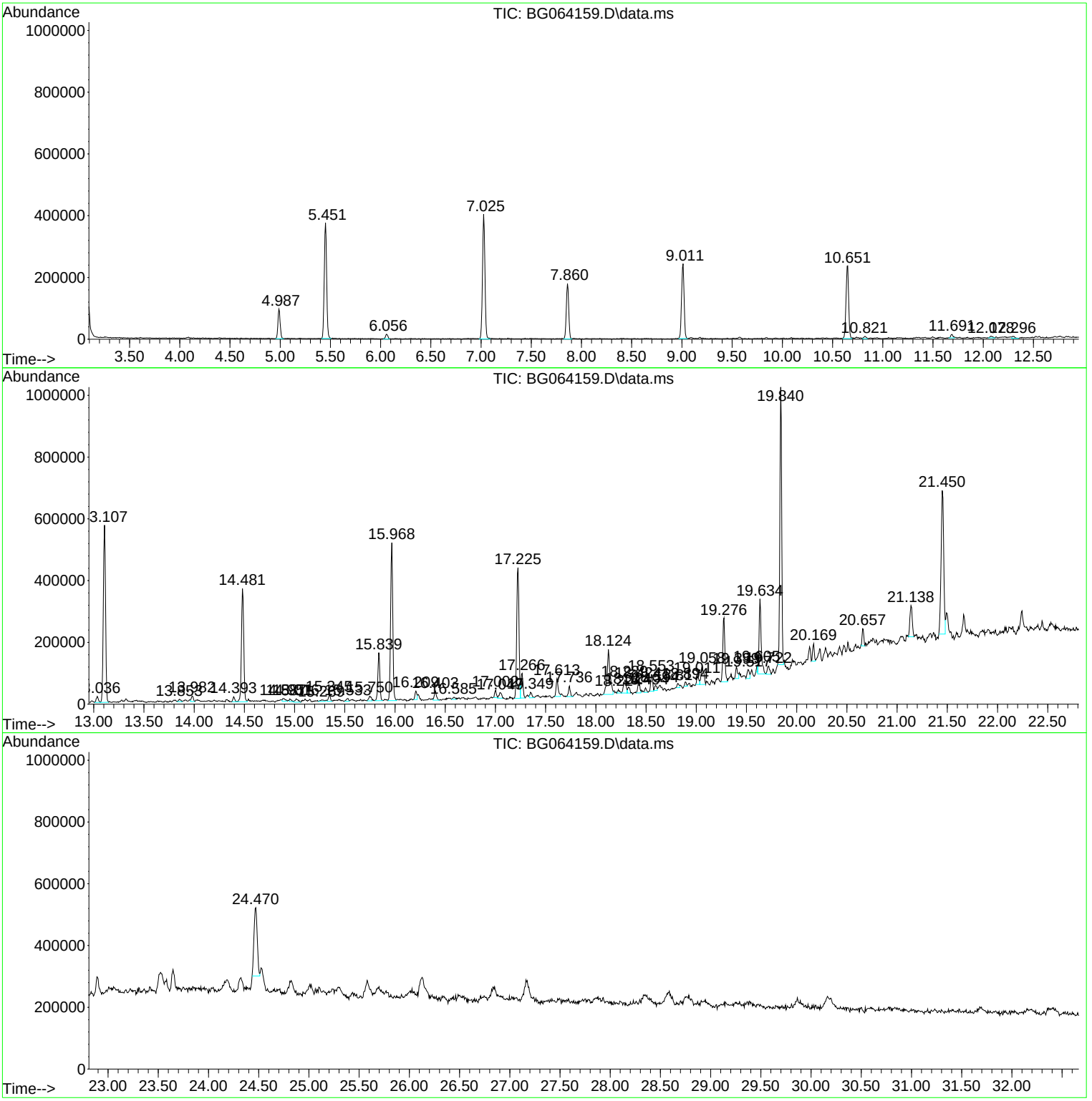
ClientSampleId :
HR-02-040125

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 : BG064159.D
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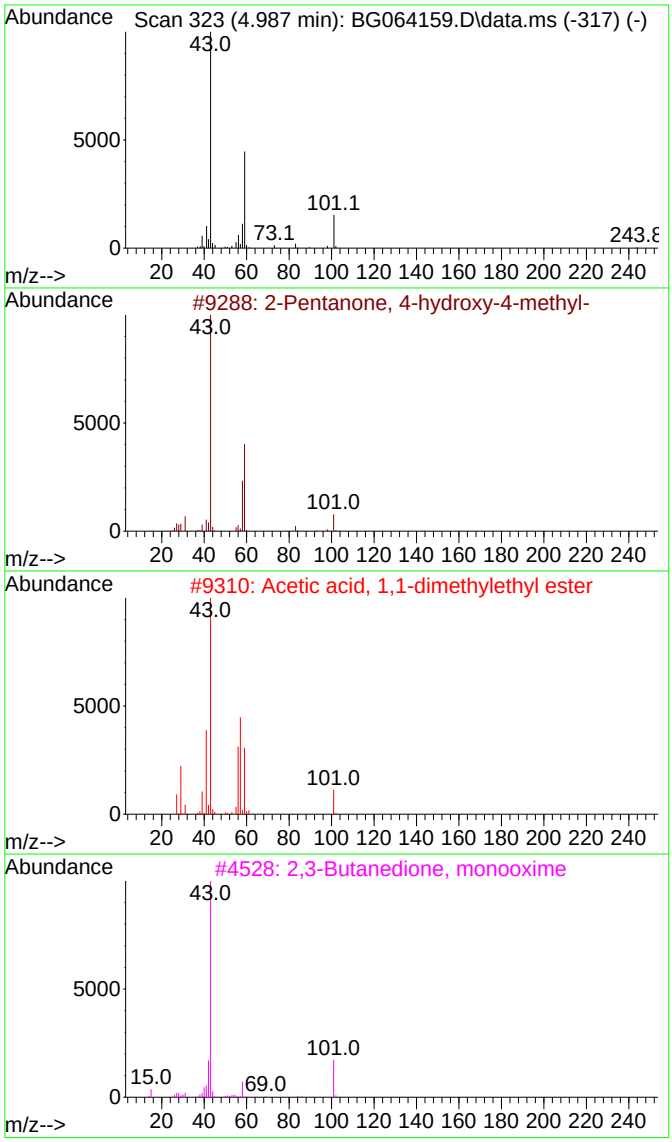
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

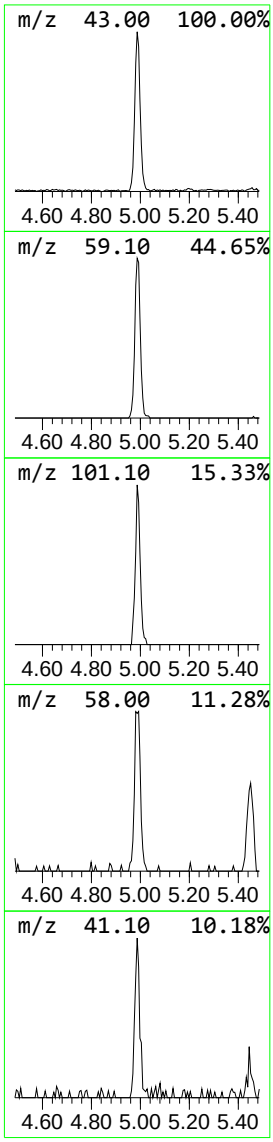
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	10.16 ng	150100	1,4-Dichlorobenzene-d4	7.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9





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Data File : BG064159.D
Acq On : 2 Apr 2025 19:04
Operator : RC/JU
Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

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

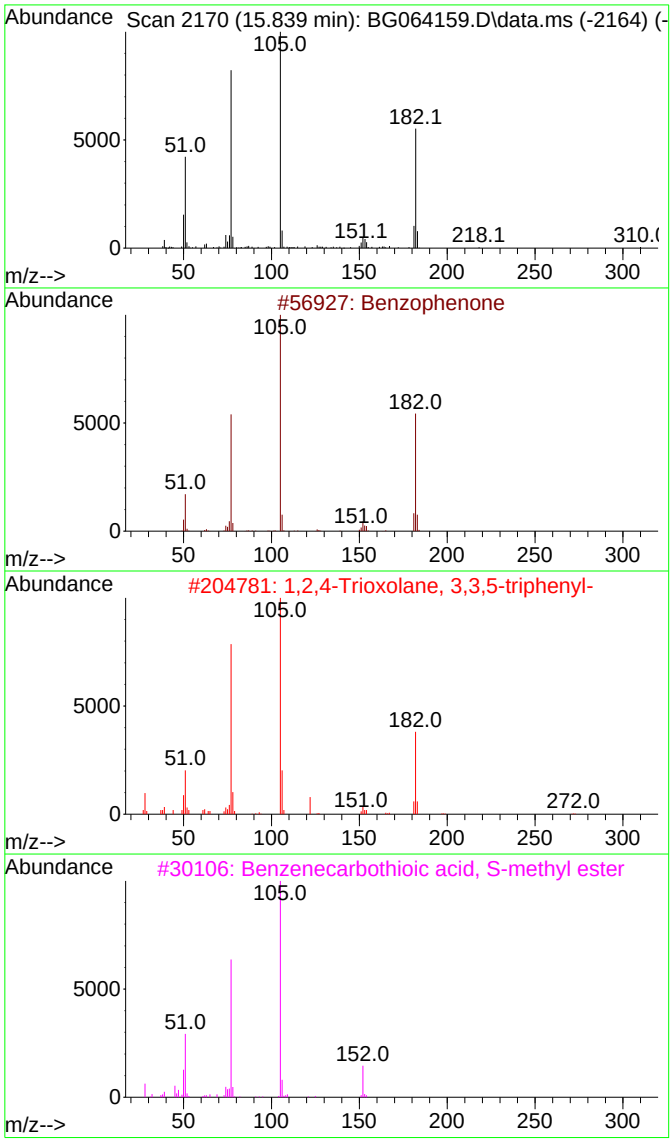
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

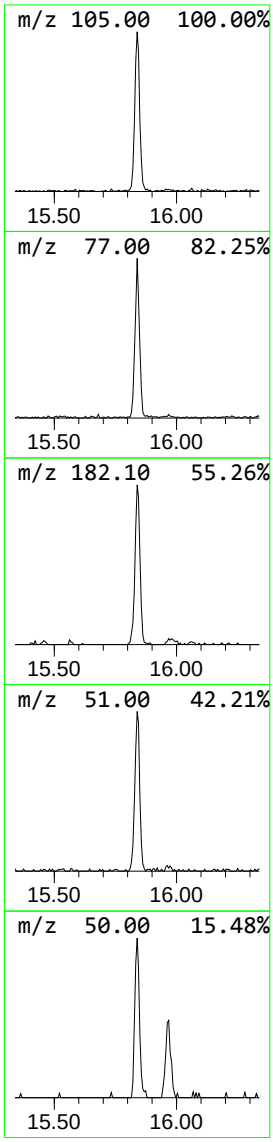
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	7.42 ng	215835	Acenaphthene-d10	14.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
4	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	53
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064159.D
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Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

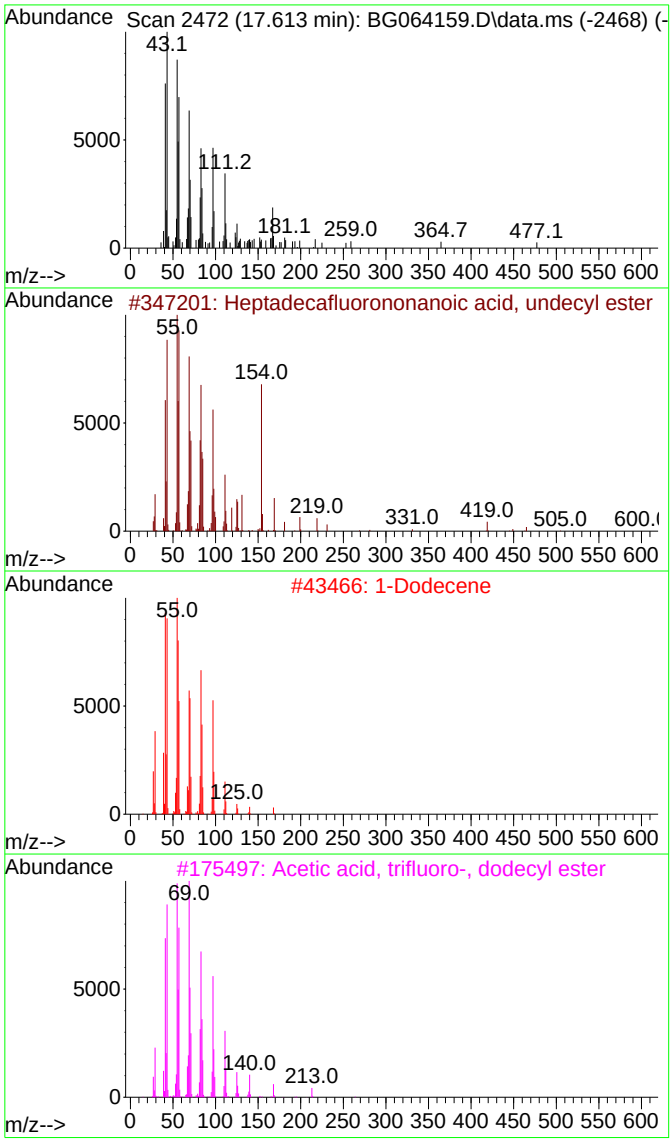
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

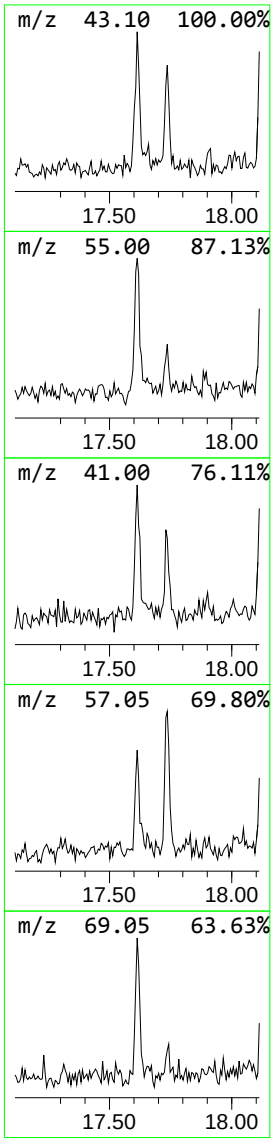
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecafluorononanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.613	2.48 ng	82516	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecafluorononanoic acid, un...	618	C20H23F17O2	1000356-02-7	83
2	1-Dodecene	168	C12H24	000112-41-4	81
3	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	74
4	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	74
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
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Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

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

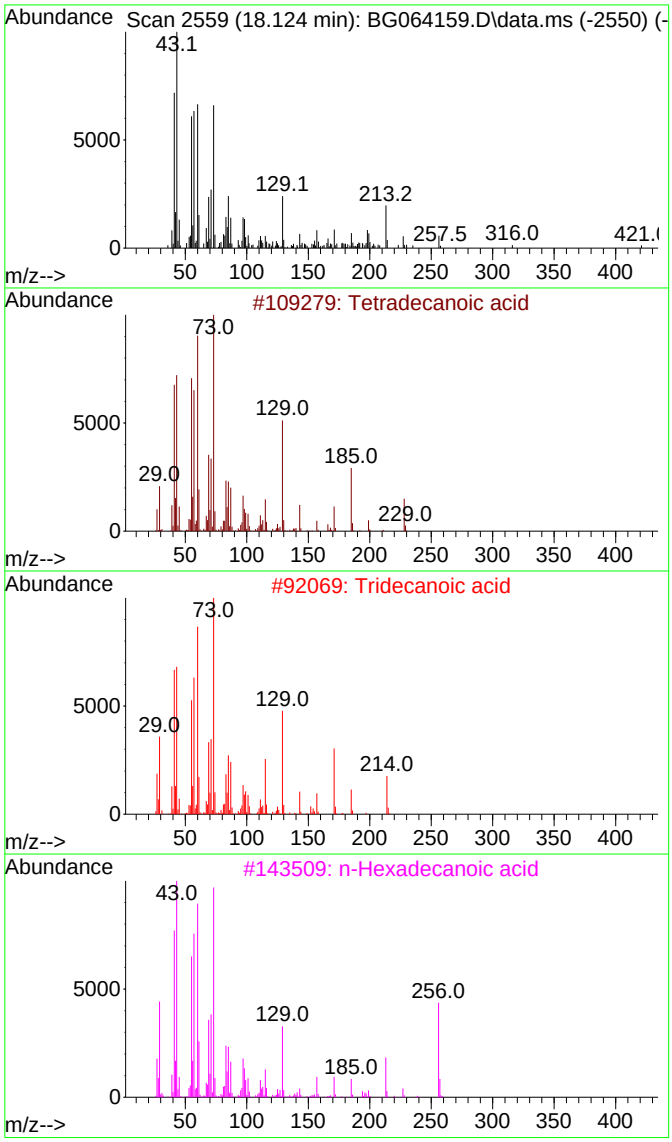
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

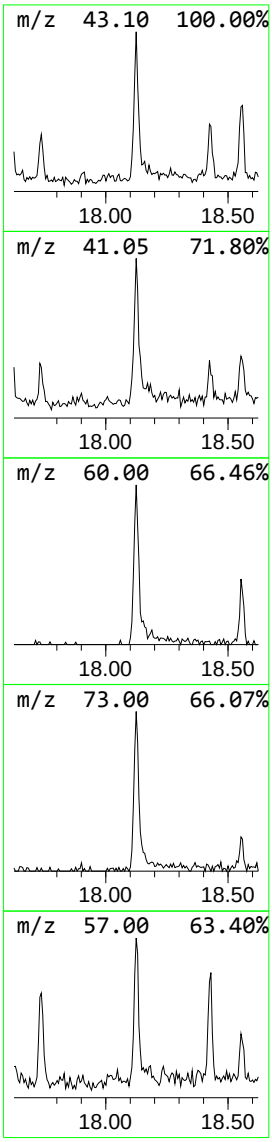
****

Peak Number 4 Tetradecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.124	8.81 ng	292941	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

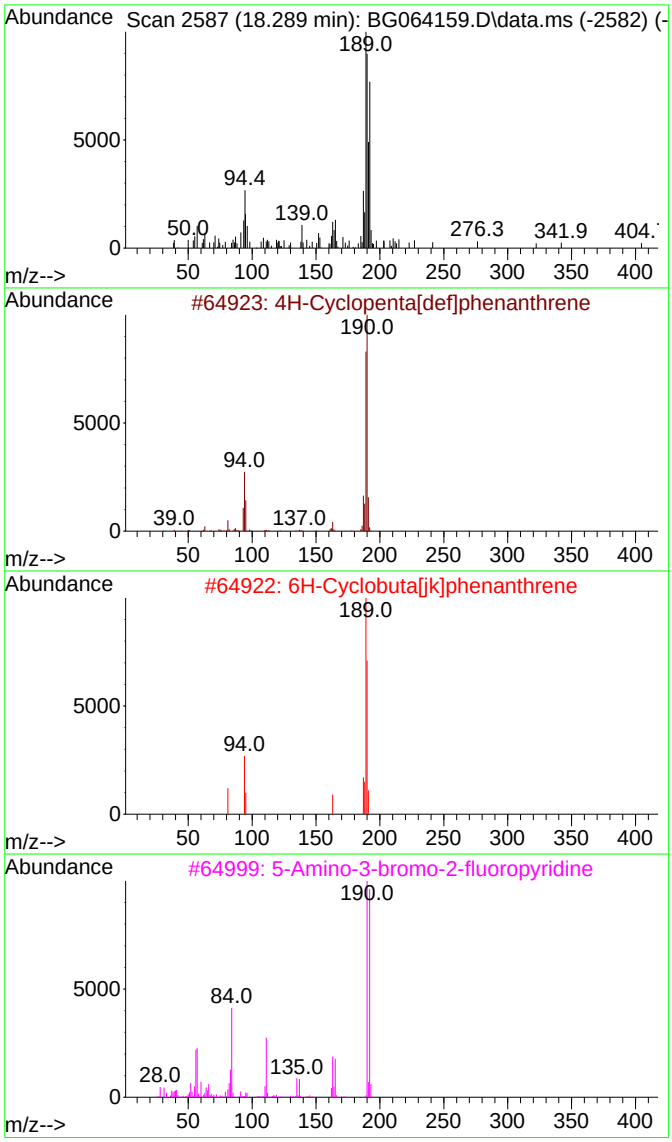
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

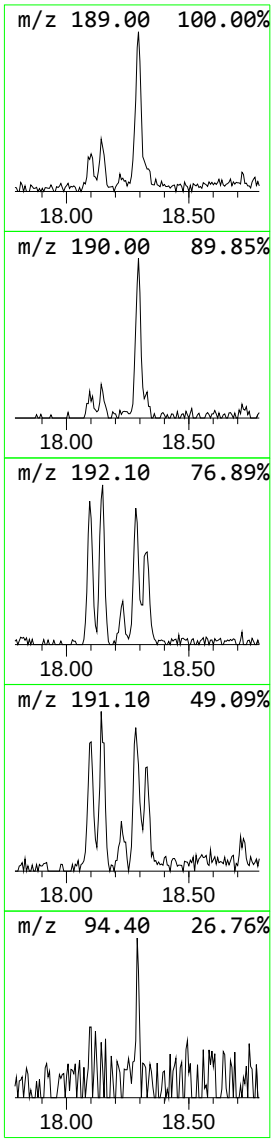
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.289	2.34 ng	77845	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
3	5-Amino-3-bromo-2-fluoropyridine	190	C5H4BrFN2	209328-99-4	38
4	4-Amino-3,5-dichloro-2,6-lutidine	190	C7H8Cl2N2	050978-40-0	38
5	2-Amino-5-bromo-3-fluoropyridine	190	C5H4BrFN2	748812-37-5	35





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

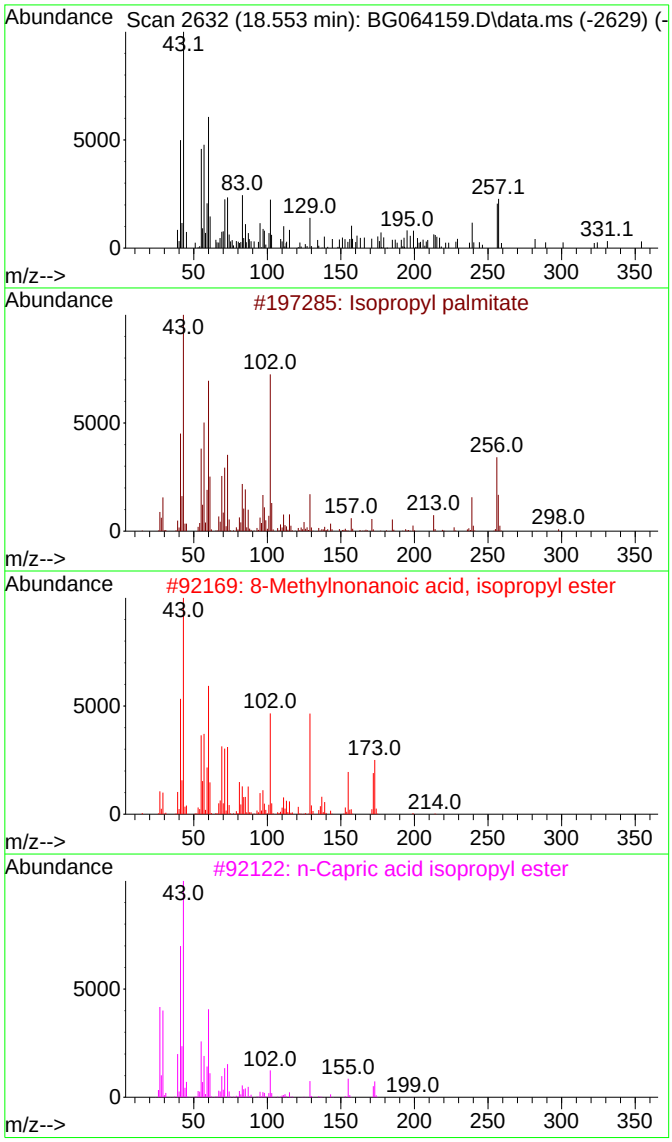
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

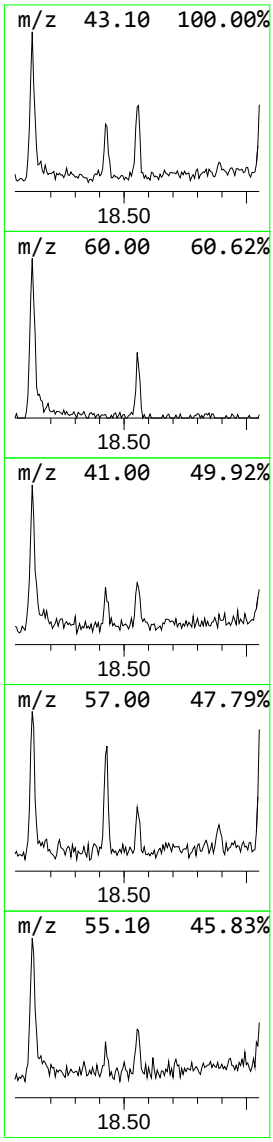
****

Peak Number 6 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.553	2.18 ng	72513	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	59
2	8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	49
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47
4	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	47
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42





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Sample : Q1685-01 2X
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ALS Vial : 14 Sample Multiplier: 1

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

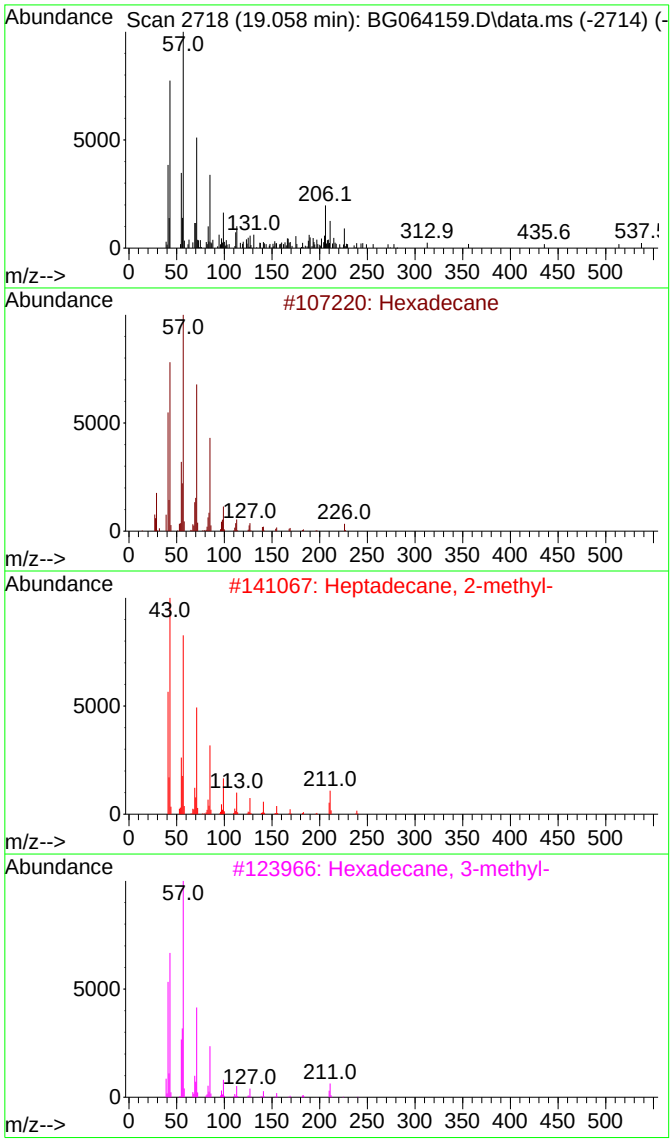
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

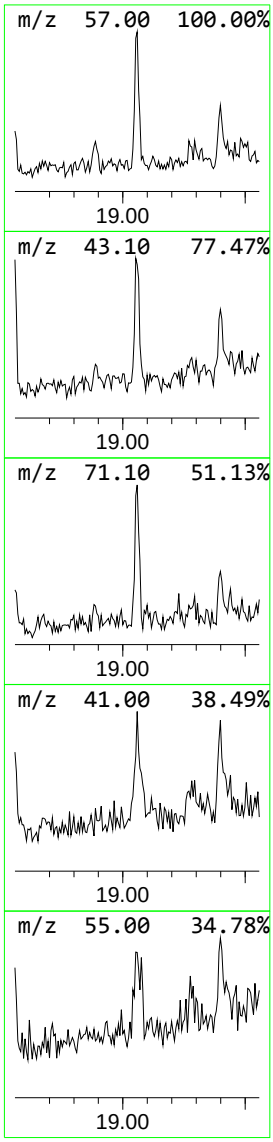
****

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.058	3.33 ng	110668	Phenanthrene-d10	17.225

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	60
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	53
3	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	49
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	46
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	45





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Data File : BG064159.D
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Instrument :
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ClientSampleId :
HR-02-040125

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

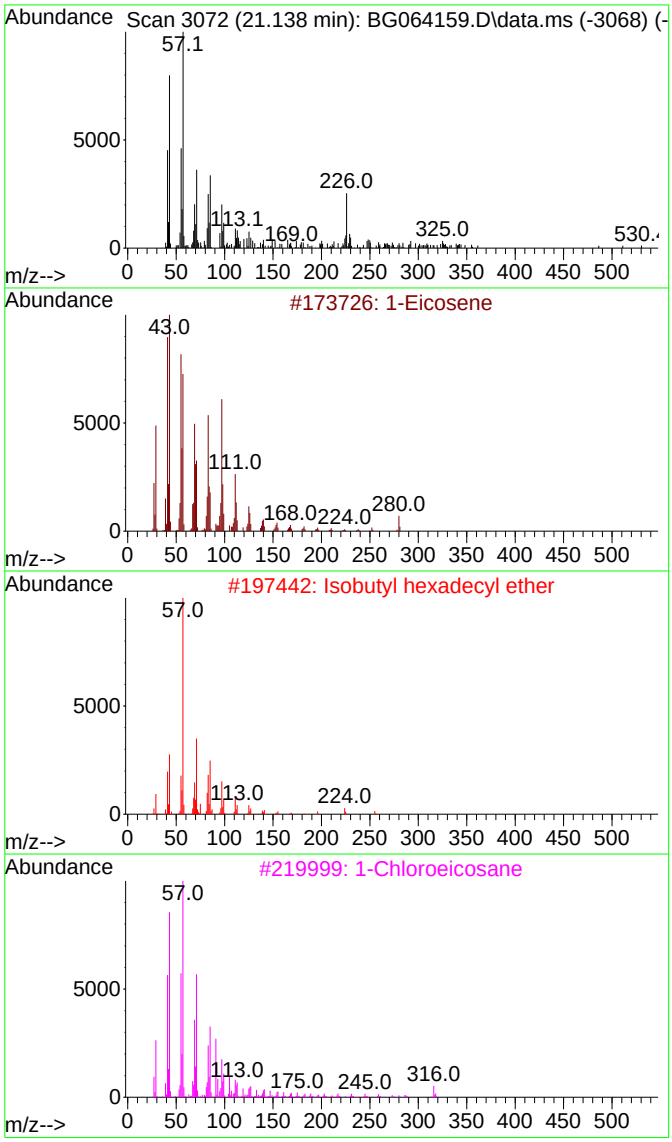
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

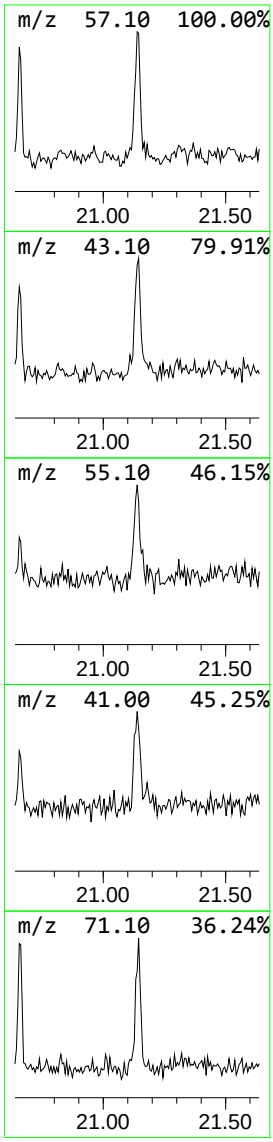
****

Peak Number 8 1-Eicosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.138	3.88 ng	162505	Chrysene-d12	21.450

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	56
2	Isobutyl hexadecyl ether	298	C20H42O	1000406-32-8	38
3	1-Chloroeicosane	316	C20H41Cl	042217-02-7	38
4	Isobutyl tetradecyl ether	270	C18H38O	1000406-32-7	38
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040225\
Data File : BG064159.D
Acq On : 2 Apr 2025 19:04
Operator : RC/JU
Sample : Q1685-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-040125

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
2-Pentanone, 4-...	4.987	10.2	ng	150100	1	7.860	295398	20.0
Benzophenone	15.839	7.4	ng	215835	3	14.481	581834	20.0
Heptadecafluoro...	17.613	2.5	ng	82516	4	17.225	665123	20.0
Tetradecanoic acid	18.124	8.8	ng	292941	4	17.225	665123	20.0
4H-Cyclopenta[d...	18.289	2.3	ng	77845	4	17.225	665123	20.0
Isopropyl palmi...	18.553	2.2	ng	72513	4	17.225	665123	20.0
Hexadecane	19.058	3.3	ng	110668	4	17.225	665123	20.0
1-Eicosene	21.138	3.9	ng	162505	5	21.450	837802	20.0