LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

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-BG102422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.857	93	97	109	rVB	13307	23407	1.52%	0.214%
2	5.315	338	345	358	rBV	91296	144427	9.36%	1.319%
3	5.796	420	427	435	rBV	477134	767888	49.75%	7.013%
4	7.412	694	702	710	rBV	495577	835002	54.10%	7.626%
5	8.270	838	848	855	rBV	152073	257302	16.67%	2.350%
6	9.445	1038	1048	1061	rBV	294636	532560	34.50%	4.864%
7	11.102	1322	1330	1337	rBV	210474	375331	24.32%	3.428%
8	13.511	1733	1740	1749	rVB	712319	1084655	70.27%	9.906%
9	14.204	1852	1858	1863	rBV3	9087	15481	1.00%	0.141%
10	14.880	1960	1973	1981	rBV	329456	527257	34.16%	4.815%
11	16.360	2219	2225	2234	rBV	522372	811630	52.58%	7.412%
12	16.572	2258	2261	2267	rVB3	13590	18850	1.22%	0.172%
13	17.336	2387	2391	2397	rBV2	9717	16099	1.04%	0.147%
14	17.618	2431	2439	2443	rBV	423192	649606	42.09%	5.933%
15	17.659	2443	2446	2452	rVB	42471	57396	3.72%	0.524%
16	18.470	2579	2584	2590	rBV3	46927	94856	6.15%	0.866%
17	18.534	2591	2595	2600	rVB2	24833	42530	2.76%	0.388%
18	18.670	2613	2618	2622	rBV3	16833	27975	1.81%	0.255%
19	18.969	2664	2669	2672	rBV3	11630	16382	1.06%	0.150%
20	19.010	2672	2676	2684	rVB8	7900	15565	1.01%	0.142%
21	19.380	2734	2739	2745	rBV3	26301	43974	2.85%	0.402%
22	19.527	2758	2764	2769	rBV7	11071	22249	1.44%	0.203%
23	19.645	2779	2784	2790	rVB	89851	125592	8.14%	1.147%
24	19.721	2790	2797	2804	rBV10	14735	38405	2.49%	0.351%
25	19.944	2831	2835	2837	rVV2	12427	18996	1.23%	0.173%
26	20.003	2841	2845	2851	rVV	77780	126255	8.18%	1.153%
27	20.068	2853	2856	2862	rVB5	12494	17956	1.16%	0.164%
28	20.191	2871	2877	2882	rVB	1180193	1543549	100.00%	14.097%
29	20.326	2892	2900	2905	rBV7	10600	28532	1.85%	0.261%
30	20.467	2921	2924	2932	rVB3	28344	54120	3.51%	0.494%
31	20.785	2974	2978	2983	rBV5	12692	21327	1.38%	0.195%
32	20.961	3005	3008	3013	rVB2	22297	28233	1.83%	0.258%
33	21.261	3055	3059	3067	rVB2	15453	27520	1.78%	0.251%
34	21.490	3093	3098	3105	rBV2	83093	140398	9.10%	1.282%
35	21.742	3138	3141	3146	rVB4	16107	22838	1.48%	0.209%
36	21.889	3157	3166	3172	rBV2	434148	831369	53.86%	7.593%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

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-BG102422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.936	3172	3174	3181	rVB	47024	68537	4.44%	0.626%
38	22.048	3191	3193	3198	rVB	18958	25586	1.66%	0.234%
39	22.682	3299	3301	3306	rVB	14726	17976	1.16%	0.164%
40	22.935	3340	3344	3351	rBV8	17716	35630	2.31%	0.325%
41	23.411	3418	3425	3435	rBV4	28162	68591	4.44%	0.626%
42	23.787	3484	3489	3493	rBV6	13064	25784	1.67%	0.235%
43	24.192	3552	3558	3565	rBV3	37695	118122	7.65%	1.079%
44	24.263	3565	3570	3577	rVB3	60785	140117	9.08%	1.280%
45	24.962	3684	3689	3701	rVB3	26260	76381	4.95%	0.698%
46	25.121	3711	3716	3730	rVB2	31646	83772	5.43%	0.765%
47	25.279	3733	3743	3755	rBV2	252954	762340	49.39%	6.962%
48	26.466	3937	3945	3954	rVB3	39601	121261	7.86%	1.107%

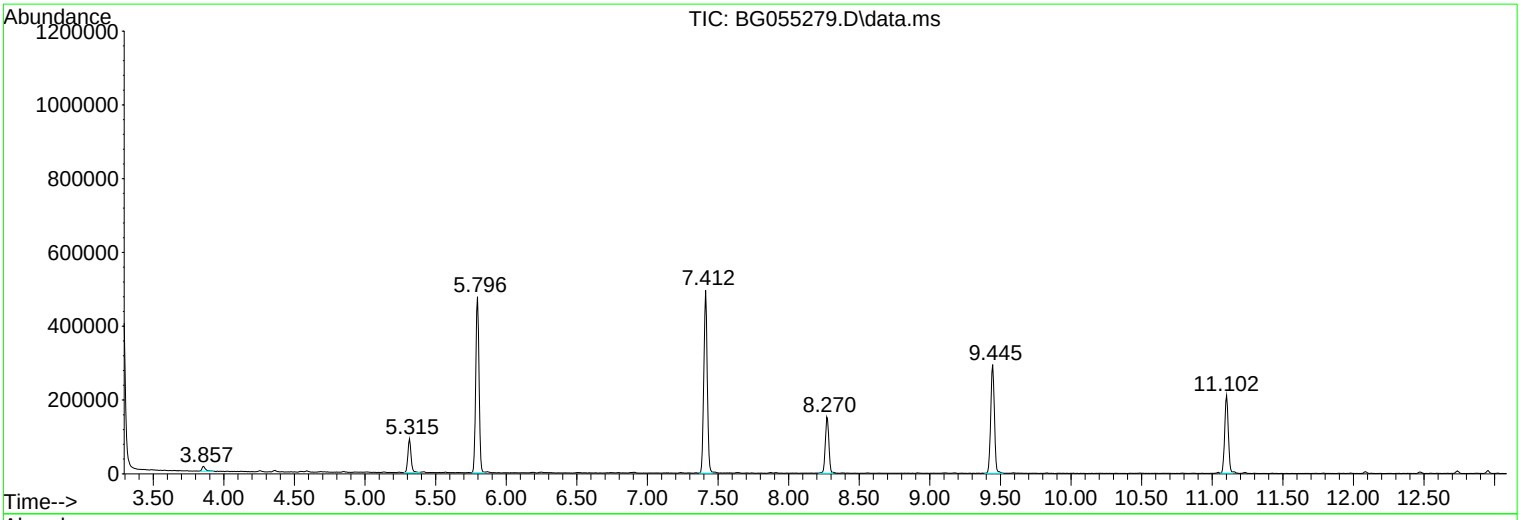
Sum of corrected areas: 10949609

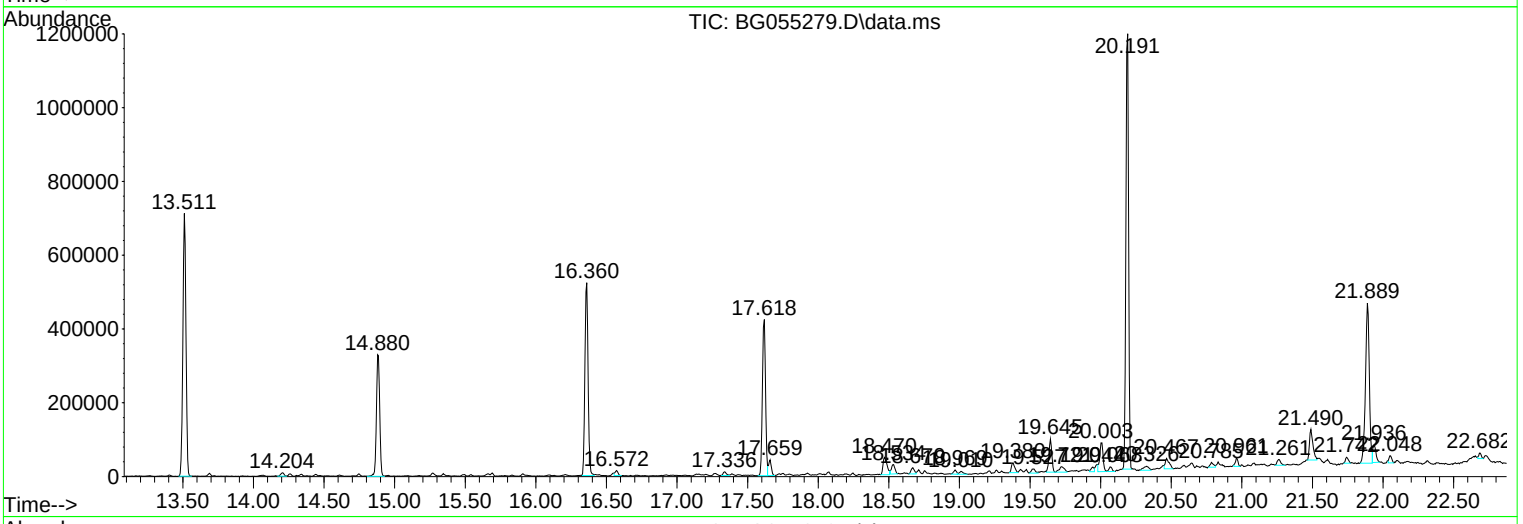
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

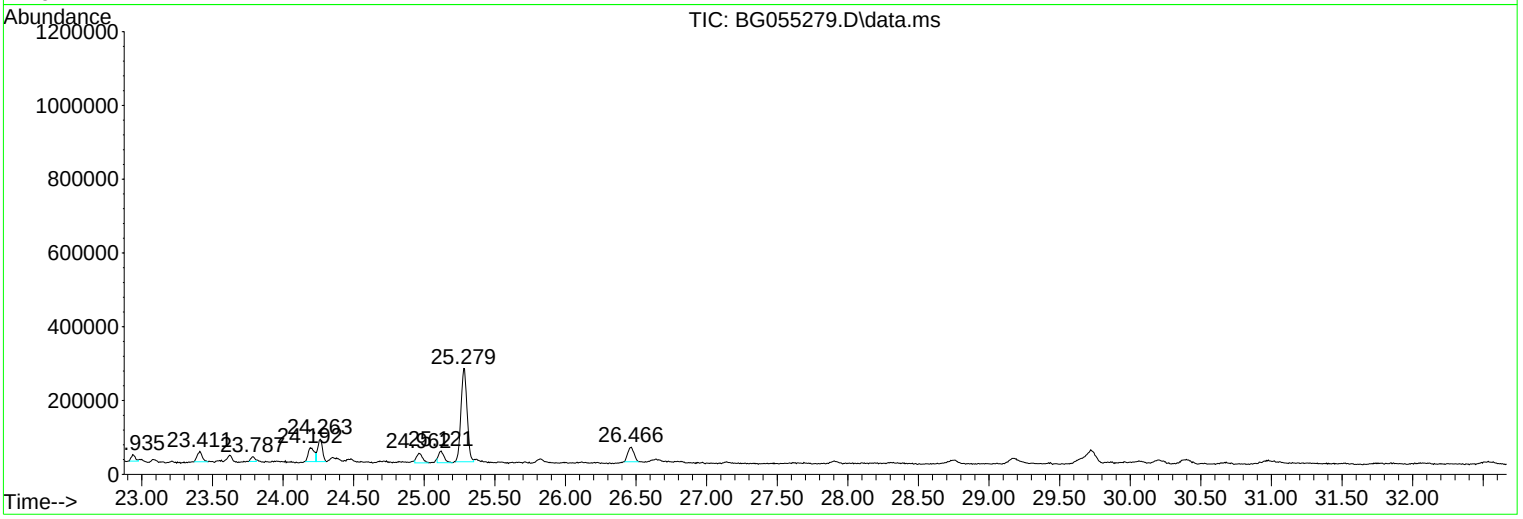
Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.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\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

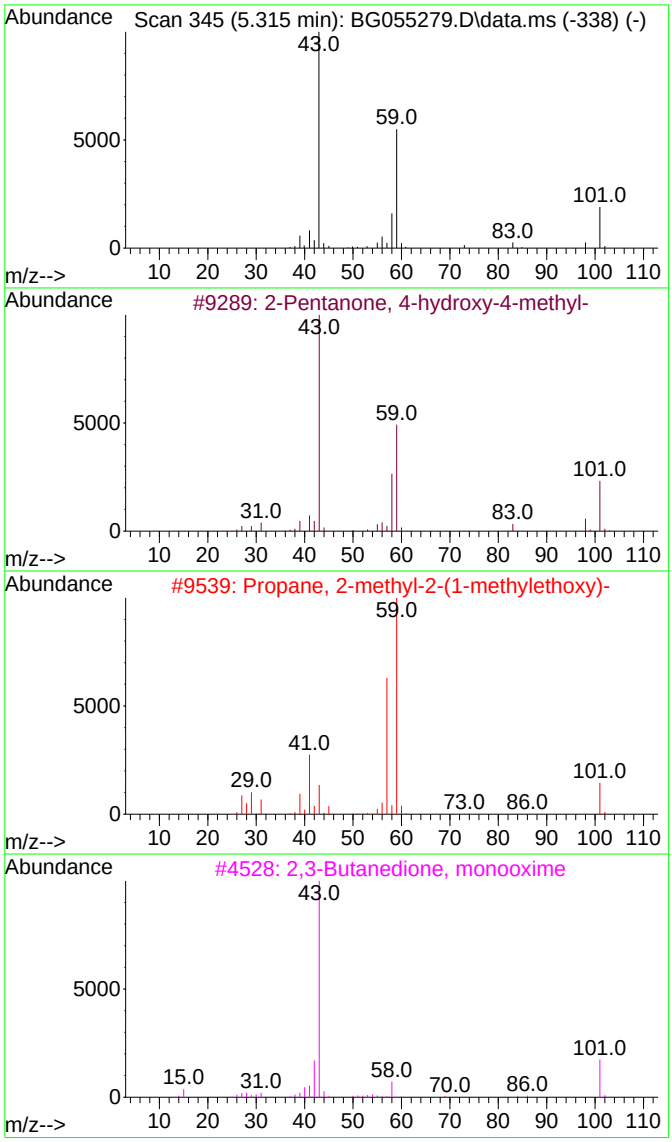
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

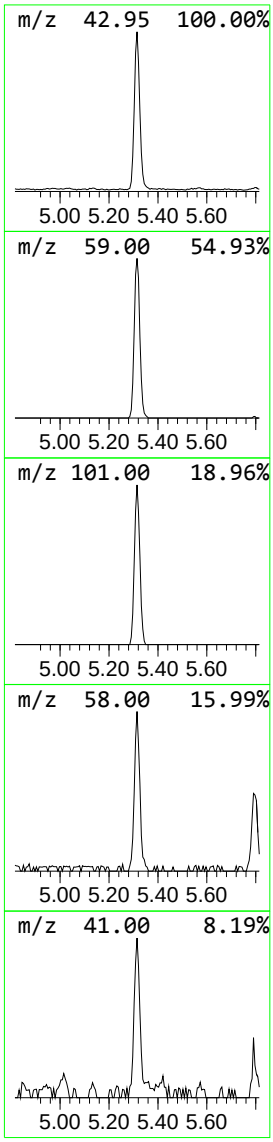
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.315	11.23 ng	144427	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1,2-Butanediol	90	C4H10O2	000584-03-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

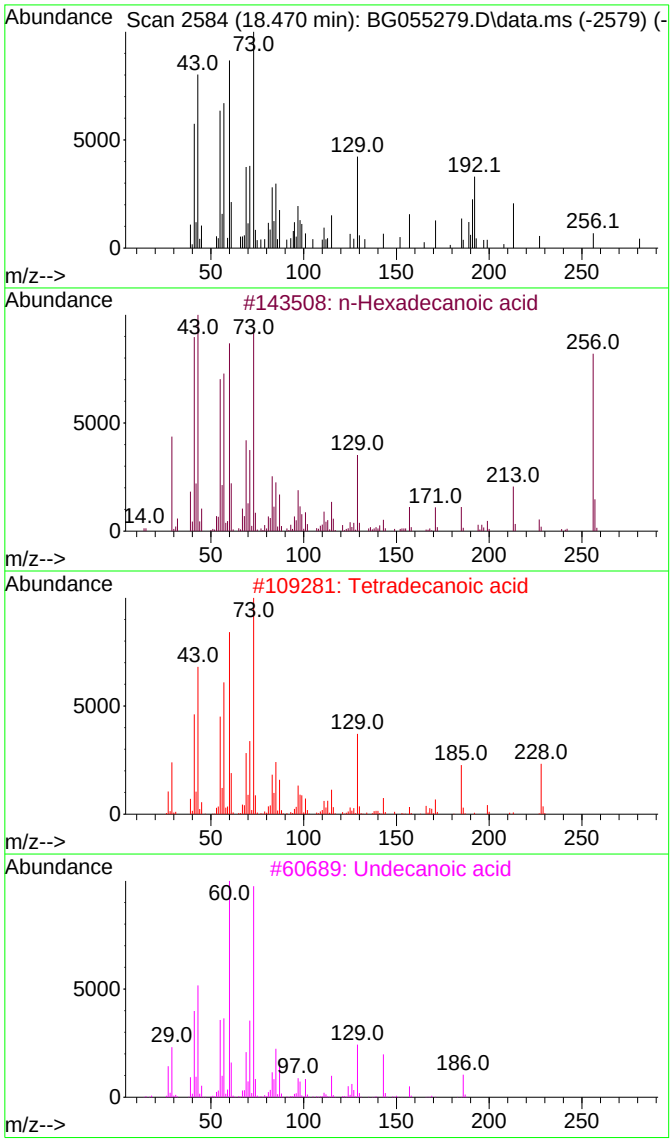
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

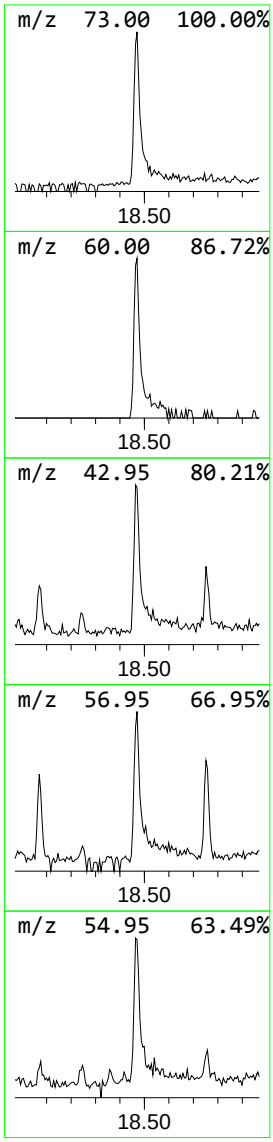
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	2.92 ng	94856	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

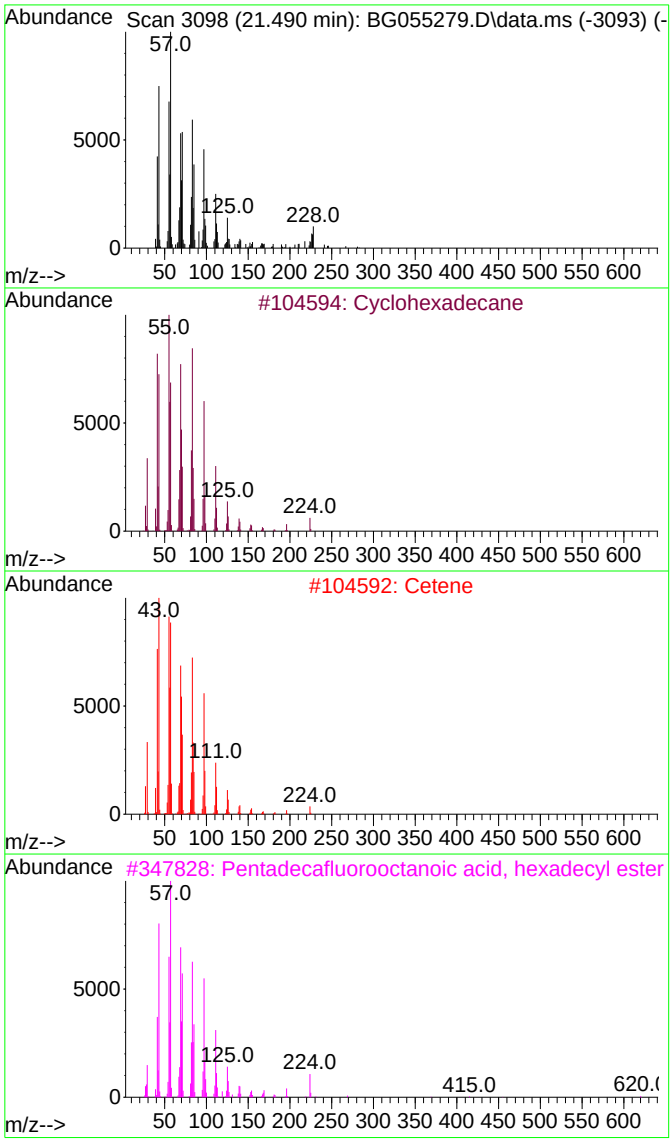
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

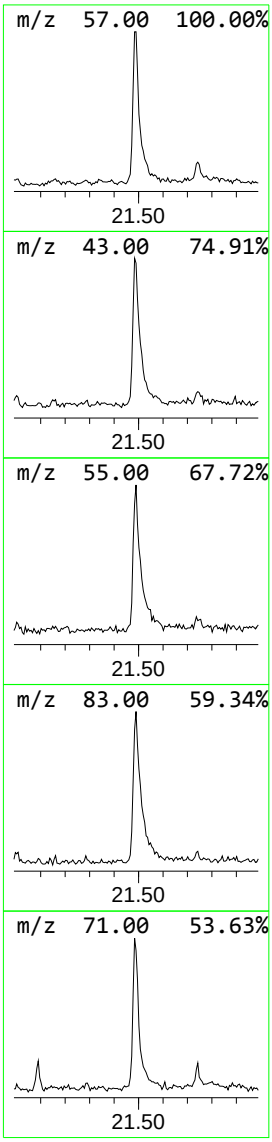
****

Peak Number 3 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	3.38 ng	140398	Chrysene-d12	21.889

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Cetene	224	C16H32	000629-73-2	95
3	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	91
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

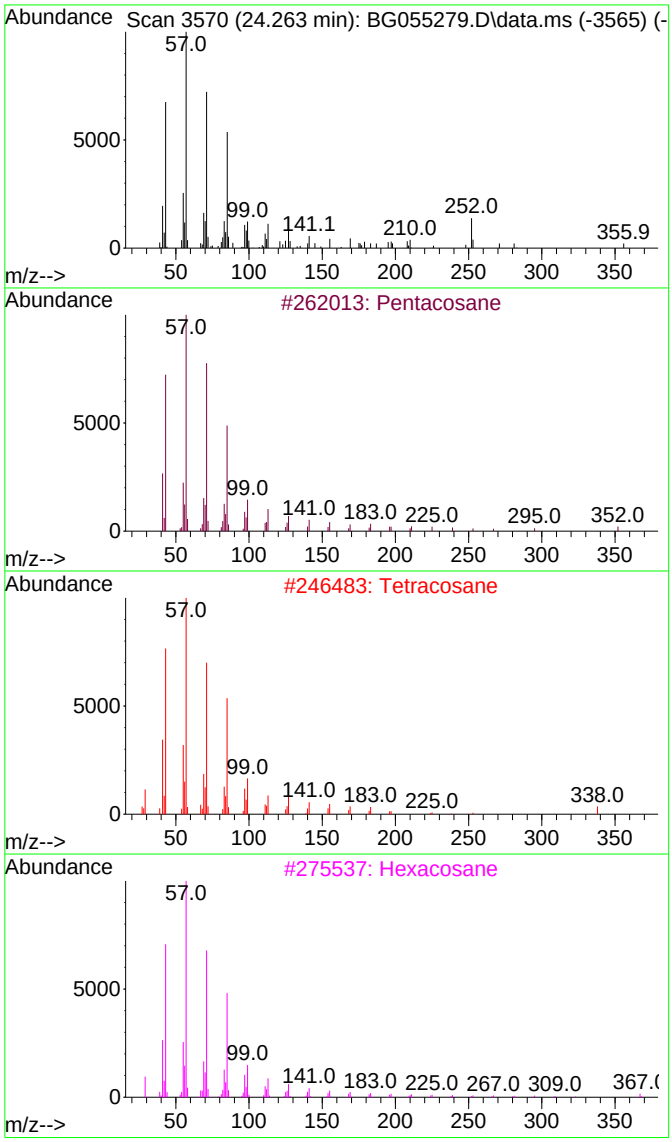
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

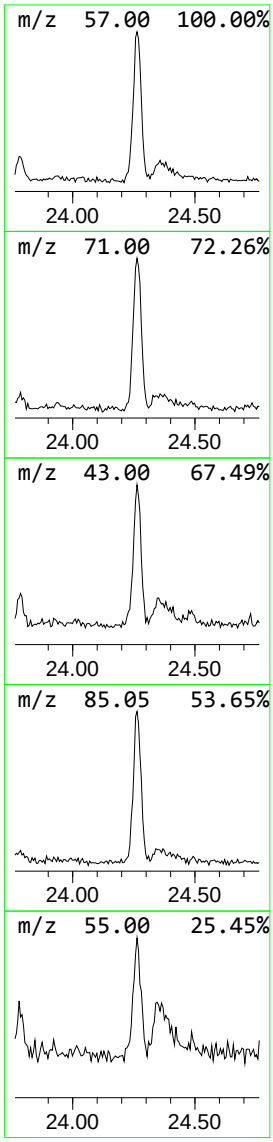
****

Peak Number 4 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.263	3.68 ng	140117	Perylene-d12	25.285

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
5	Eicosane	282	C20H42	000112-95-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

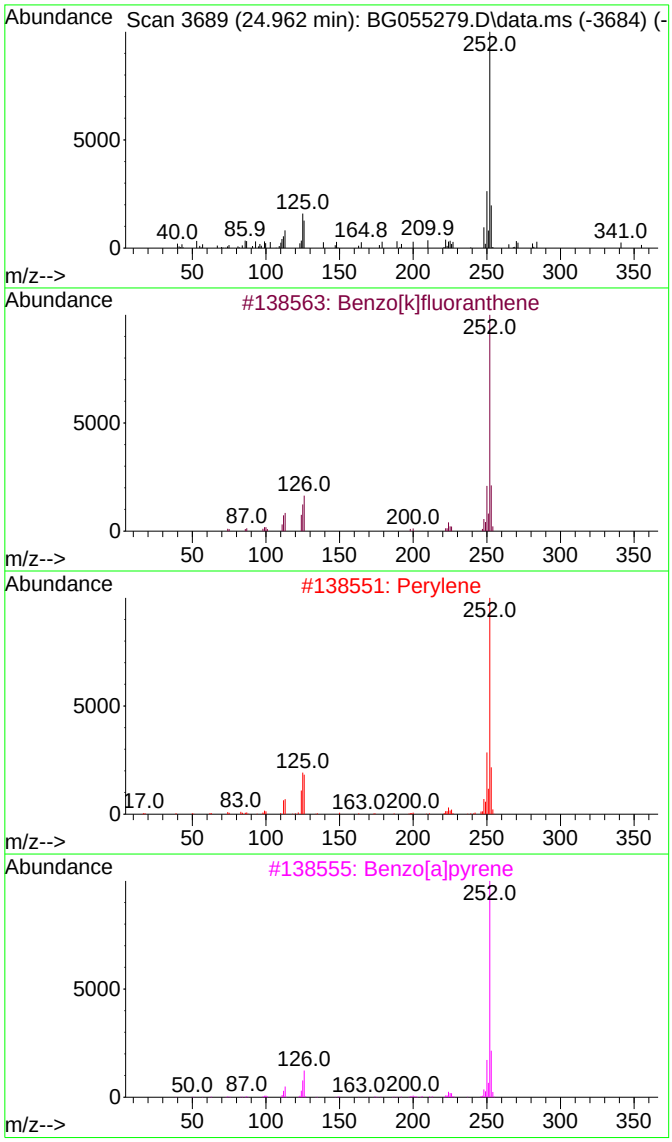
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

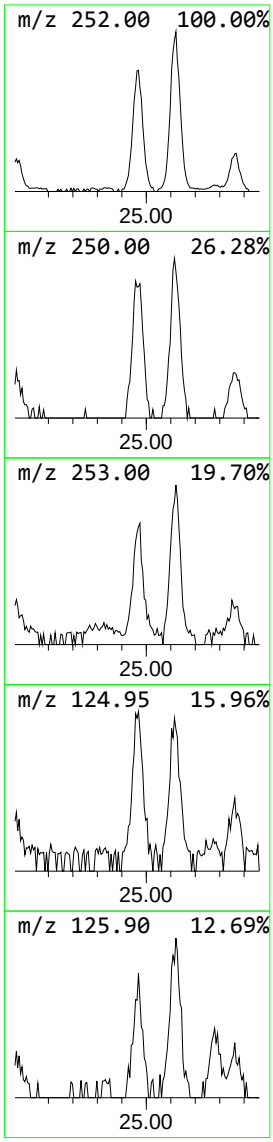
****

Peak Number 5 Benzo[k]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.962	2.00 ng	76381	Perylene-d12	25.285

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
2	Perylene	252	C20H12	000198-55-0	76
3	Benzo[a]pyrene	252	C20H12	000050-32-8	76
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	68
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	64





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Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

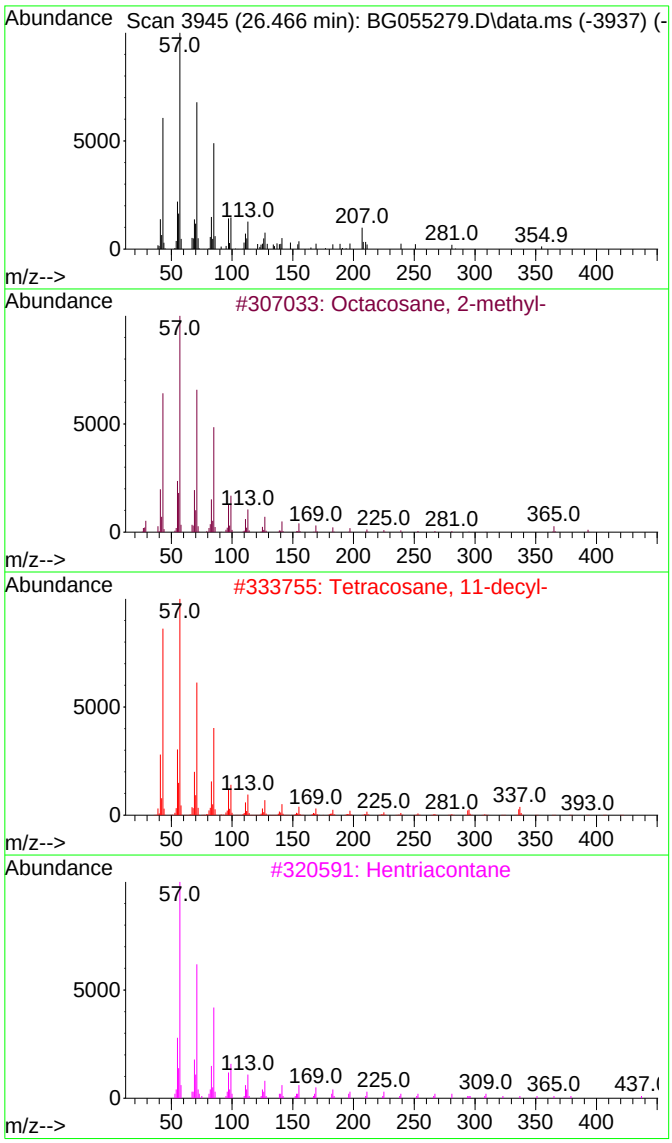
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

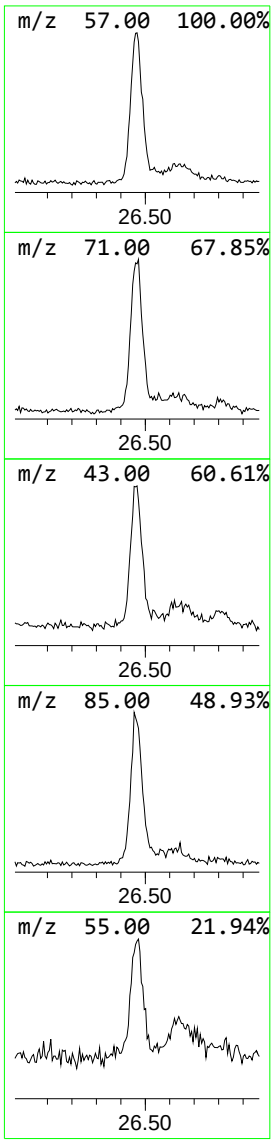
****

Peak Number 6 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.466	3.18 ng	121261	Perylene-d12	25.285

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055279.D
Acq On : 25 Oct 2022 17:06
Operator : CG/JU
Sample : N5254-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2-102122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.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-...	5.315	11.2	ng	144427	1	8.270	257302	20.0
n-Hexadecanoic ...	18.470	2.9	ng	94856	4	17.618	649606	20.0
Cyclohexadecane	21.490	3.4	ng	140398	5	21.889	831369	20.0
Pentacosane	24.263	3.7	ng	140117	6	25.285	762340	20.0
Benzo[k]fluoran...	24.962	2.0	ng	76381	6	25.285	762340	20.0
Octacosane, 2-m...	26.466	3.2	ng	121261	6	25.285	762340	20.0