LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SU-4-120222

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055896.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.594	216	222	228	rBV2	11957	19619	1.00%	0.146%
2	5.217	320	328	339	rBV	258411	409577	20.95%	3.055%
3	5.705	404	411	422	rBV	620205	1017056	52.03%	7.587%
4	6.322	510	516	523	rVB	14593	24117	1.23%	0.180%
5	7.332	679	688	702	rBV	605349	1086062	55.56%	8.101%
6	8.172	824	831	838	rBV	169021	278973	14.27%	2.081%
7	9.347	1022	1031	1041	rBV	385485	672964	34.43%	5.020%
8	10.998	1305	1312	1320	rBV	238512	417441	21.36%	3.114%
9	13.425	1715	1725	1733	rBV	1000712	1548727	79.23%	11.553%
10	14.530	1908	1913	1919	rBV	14692	25238	1.29%	0.188%
11	14.800	1953	1959	1966	rVB	350467	558723	28.58%	4.168%
12	16.145	2183	2188	2196	rVB2	17006	28288	1.45%	0.211%
13	16.286	2206	2212	2220	rBV	674537	1075865	55.04%	8.025%
14	17.544	2420	2426	2431	rBV	421160	640830	32.78%	4.780%
15	17.585	2431	2433	2439	rVB	62721	75795	3.88%	0.565%
16	17.679	2445	2449	2452	rBV	16887	26182	1.34%	0.195%
17	18.402	2568	2572	2579	rBV2	125298	220550	11.28%	1.645%
18	18.466	2579	2583	2588	rVB2	28108	48684	2.49%	0.363%
19	18.613	2602	2608	2611	rVV4	26591	60339	3.09%	0.450%
20	18.642	2611	2613	2617	rVB2	17096	20066	1.03%	0.150%
21	18.813	2638	2642	2646	rBV4	18864	25167	1.29%	0.188%
22	18.901	2654	2657	2662	rBV	15952	23511	1.20%	0.175%
23	18.954	2663	2666	2672	rVB5	14133	22966	1.17%	0.171%
24	19.195	2704	2707	2711	rBV2	16119	23508	1.20%	0.175%
25	19.312	2723	2727	2733	rBV3	35983	69669	3.56%	0.520%
26	19.465	2748	2753	2758	rBV4	24915	55292	2.83%	0.412%
27	19.582	2768	2773	2779	rVB	253592	369190	18.89%	2.754%
28	19.665	2784	2787	2795	rVB5	38817	65057	3.33%	0.485%
29	19.912	2826	2829	2831	rBV2	35543	45903	2.35%	0.342%
30	19.947	2831	2835	2842	rVB	251261	358269	18.33%	2.673%
31	20.135	2861	2867	2872	rBV	1450261	1954653	100.00%	14.581%
32	20.775	2974	2976	2984	rVB3	27878	44944	2.30%	0.335%
33	21.433	3084	3088	3095	rBV3	64379	128073	6.55%	0.955%
34	21.827	3147	3155	3160	rBV3	415970	949146	48.56%	7.080%
35	21.874	3160	3163	3174	rVB	138273	229012	11.72%	1.708%
36	23.519	3439	3443	3454	rVB2	119145	253486	12.97%	1.891%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-4-120222

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.188	3720	3727	3735	rVB	188572	532804	27.26%	3.974%

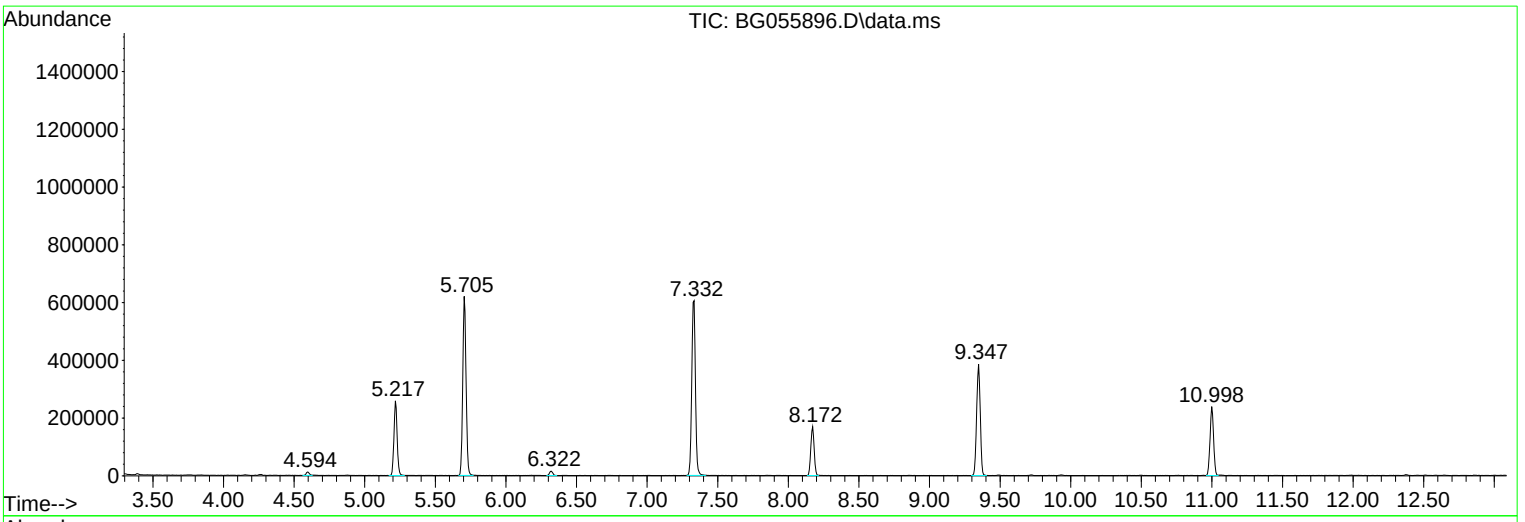
Sum of corrected areas: 13405746

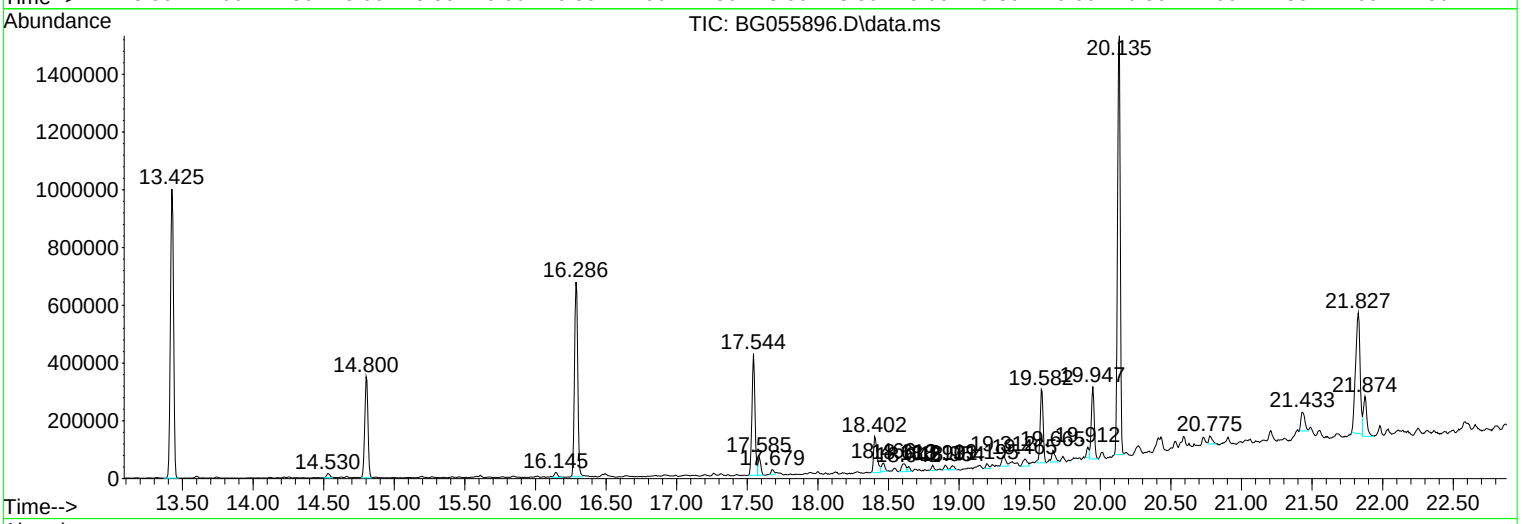
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

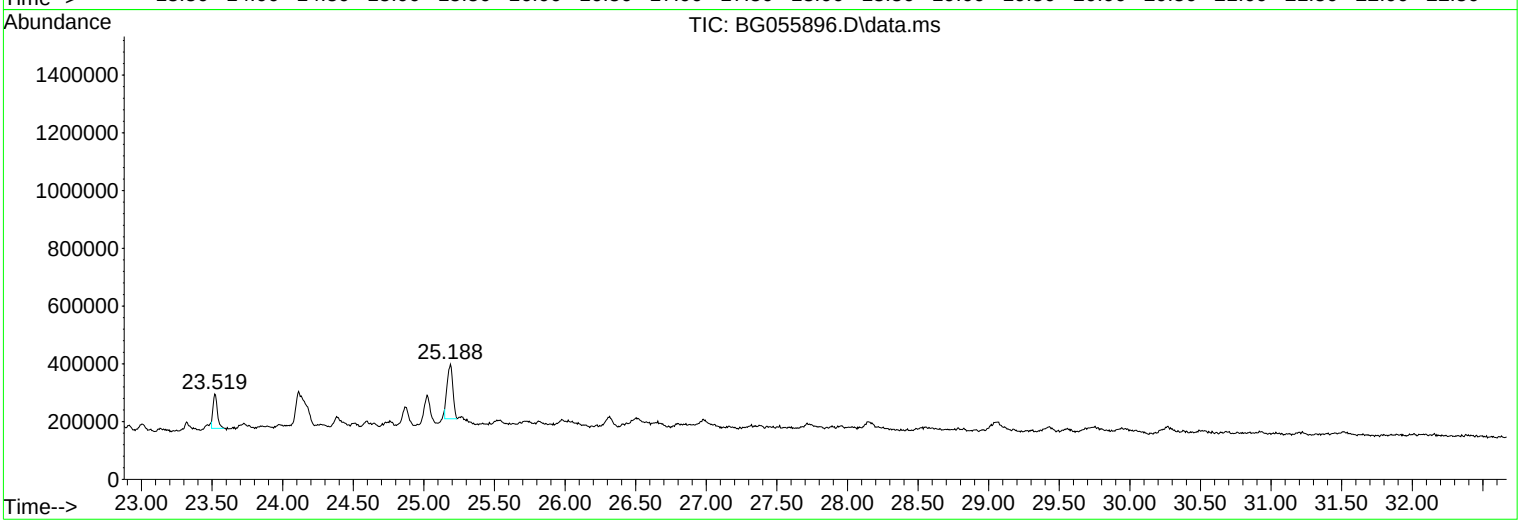
Instrument :
BNA_G
ClientSampleId :
SU-4-120222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG120522\
Data File : BG055896.D
Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-4-120222

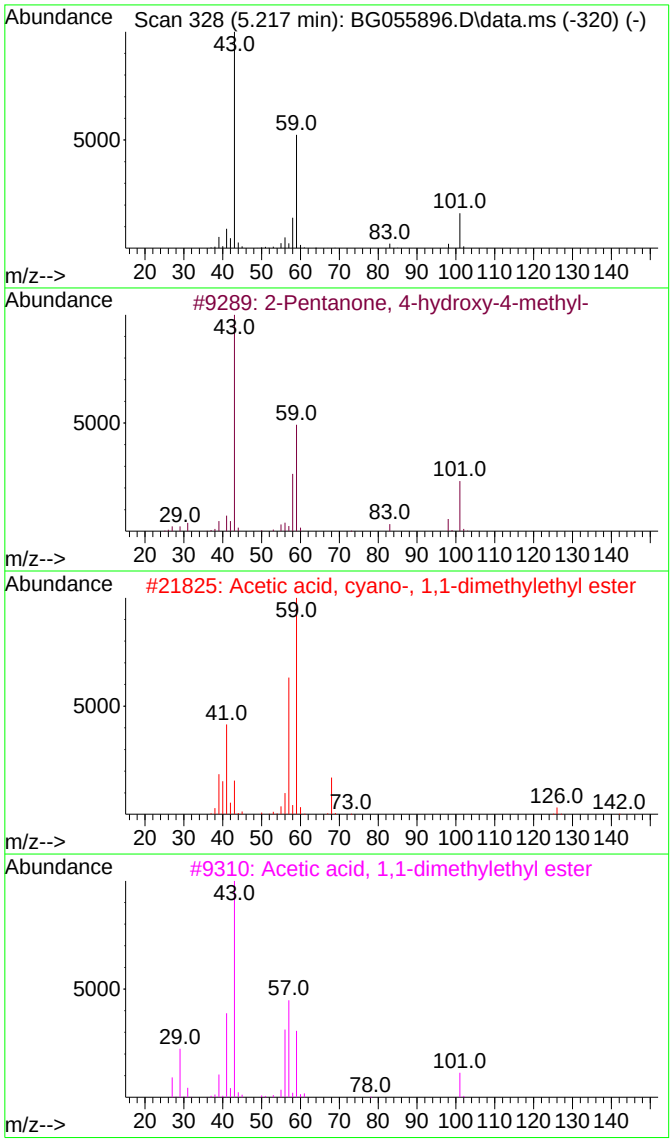
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

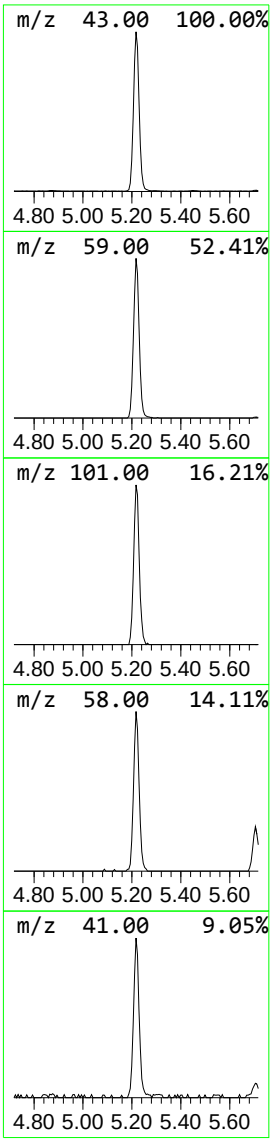
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.217	29.36 ng	409577	1,4-Dichlorobenzene-d4	8.172

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
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Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

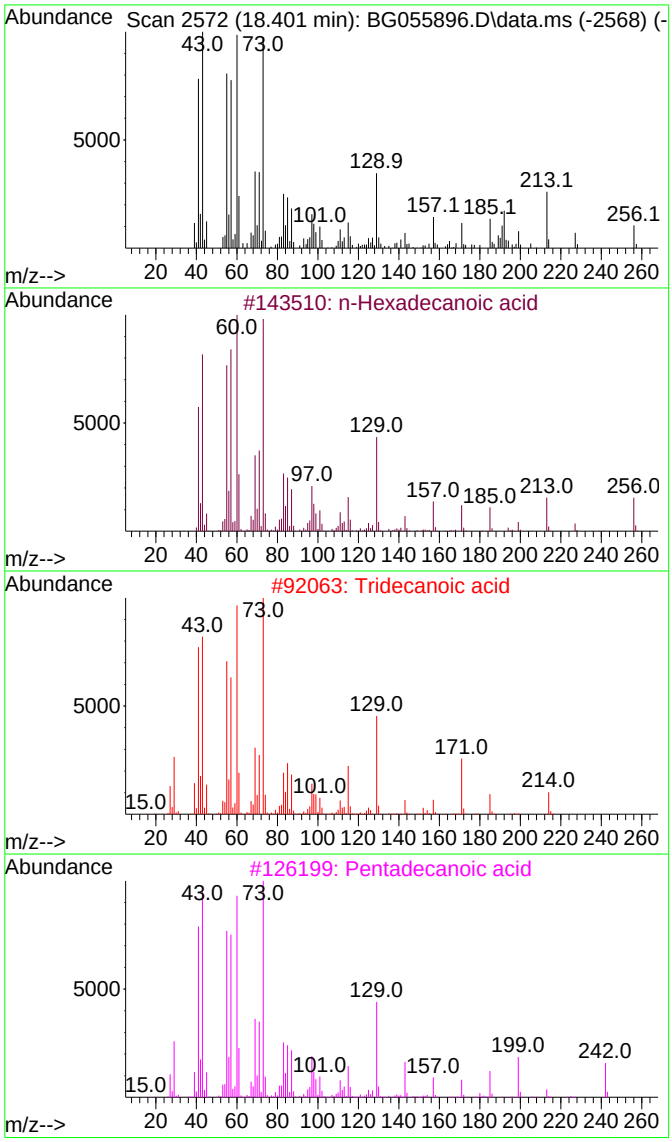
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

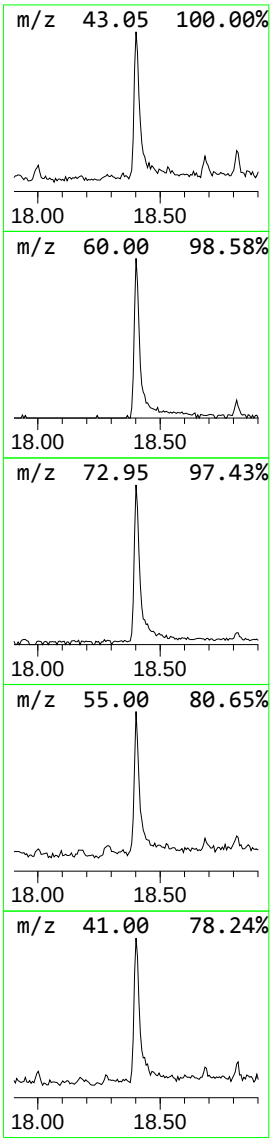
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.401	6.88 ng	220550	Phenanthrene-d10	17.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-4-120222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

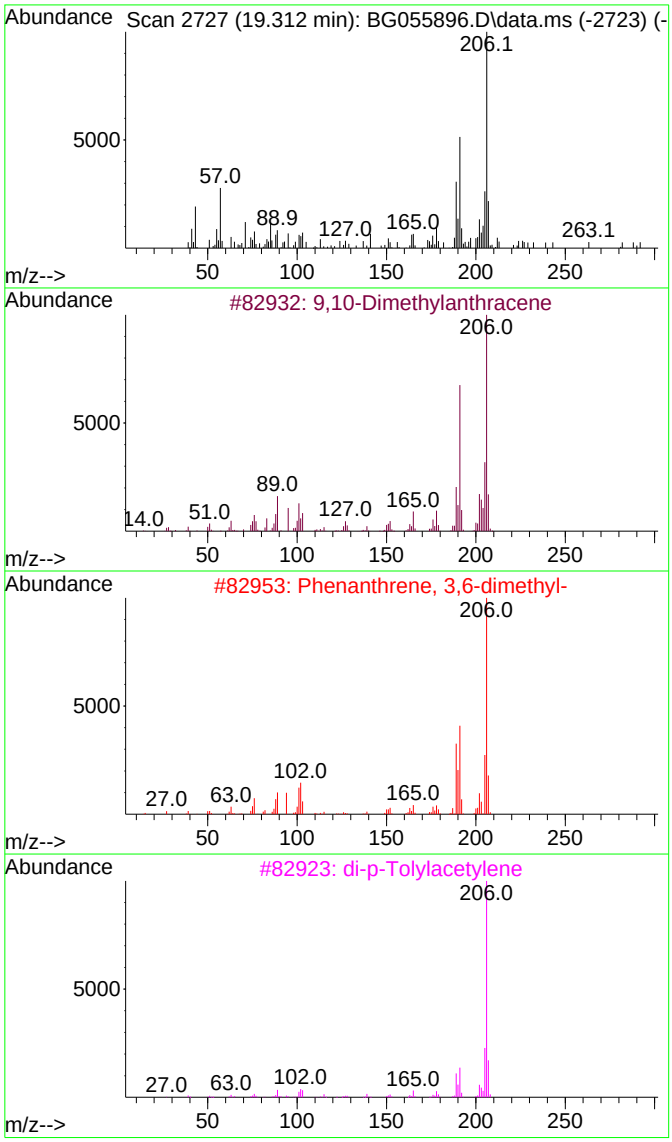
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

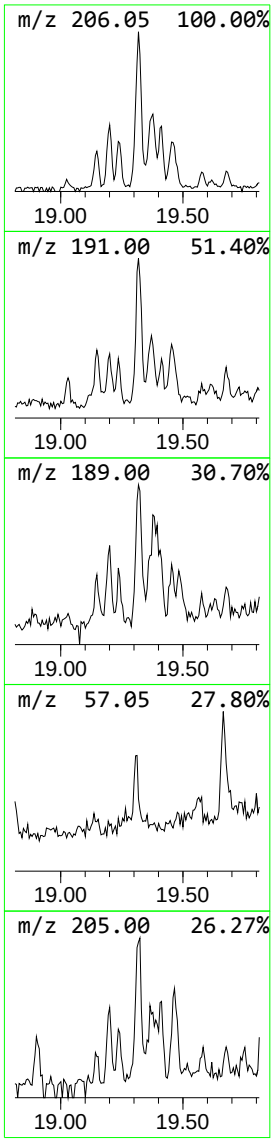
****

Peak Number 3 9,10-Dimethylanthracene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.312	2.17 ng	69669	Phenanthrene-d10	17.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	89
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	83
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	83
5	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
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Acq On : 5 Dec 2022 22:35
Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-4-120222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

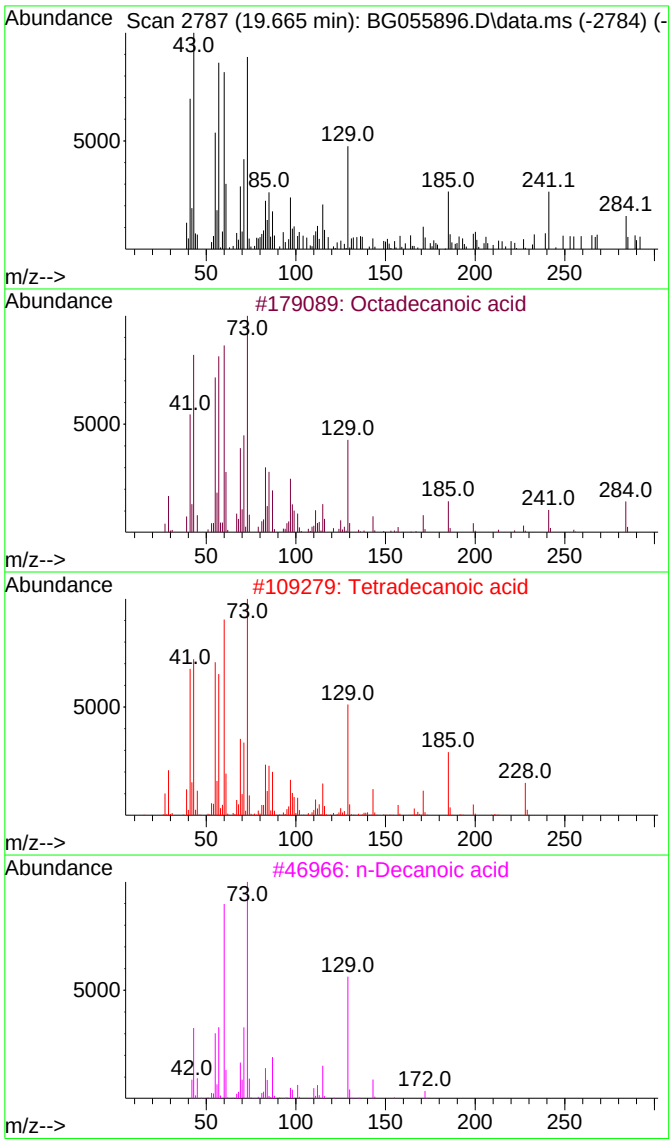
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

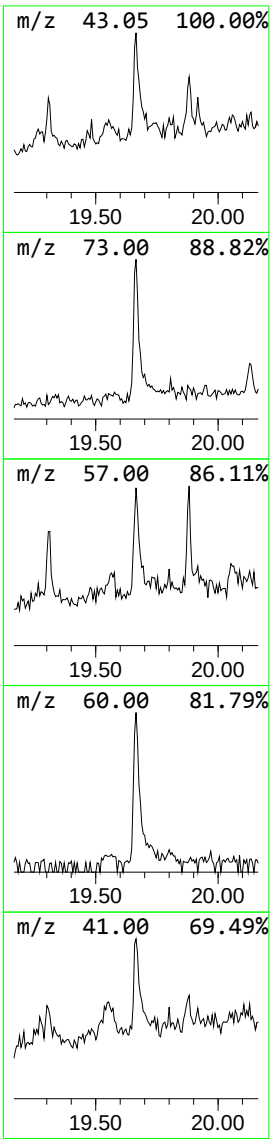
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.665	2.03 ng	65057	Phenanthrene-d10	17.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
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Operator : CG/JU
Sample : N5871-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-4-120222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

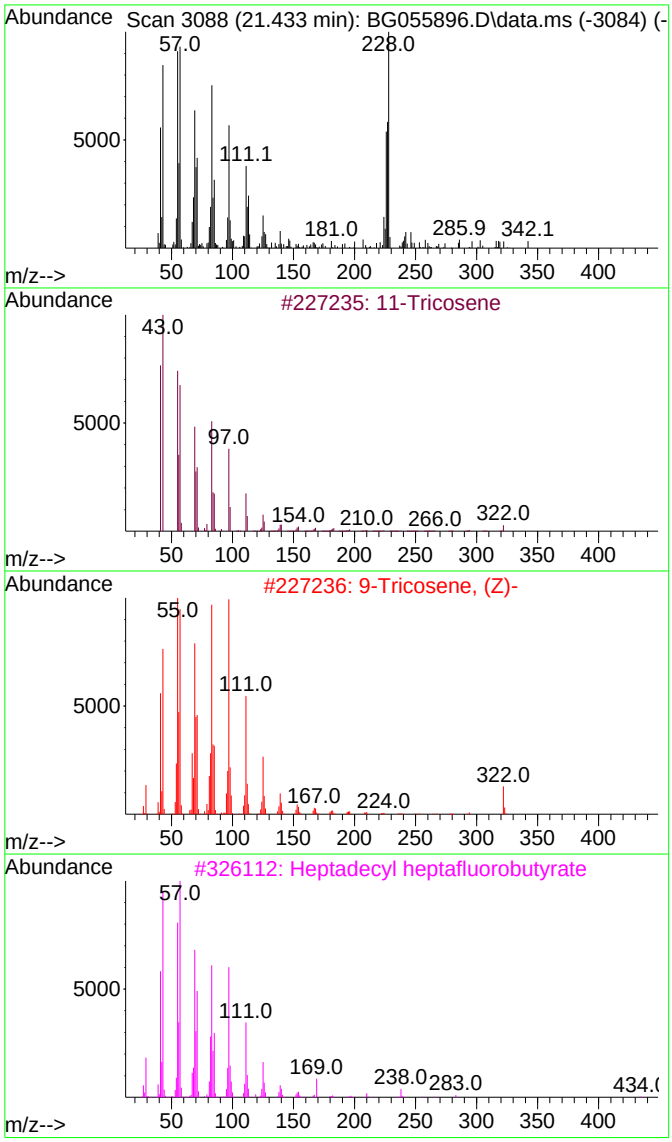
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

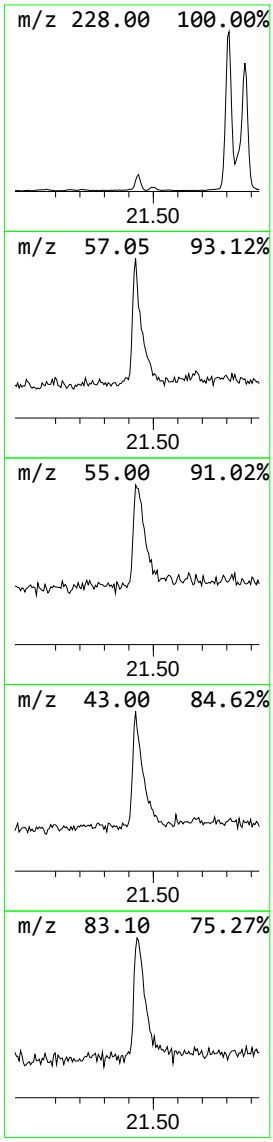
****

Peak Number 5 11-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.433	2.70 ng	128073	Chrysene-d12	21.827

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	81
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	62
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50
4	Z-8-Hexadecene	224	C16H32	1000130-87-5	49
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	46





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

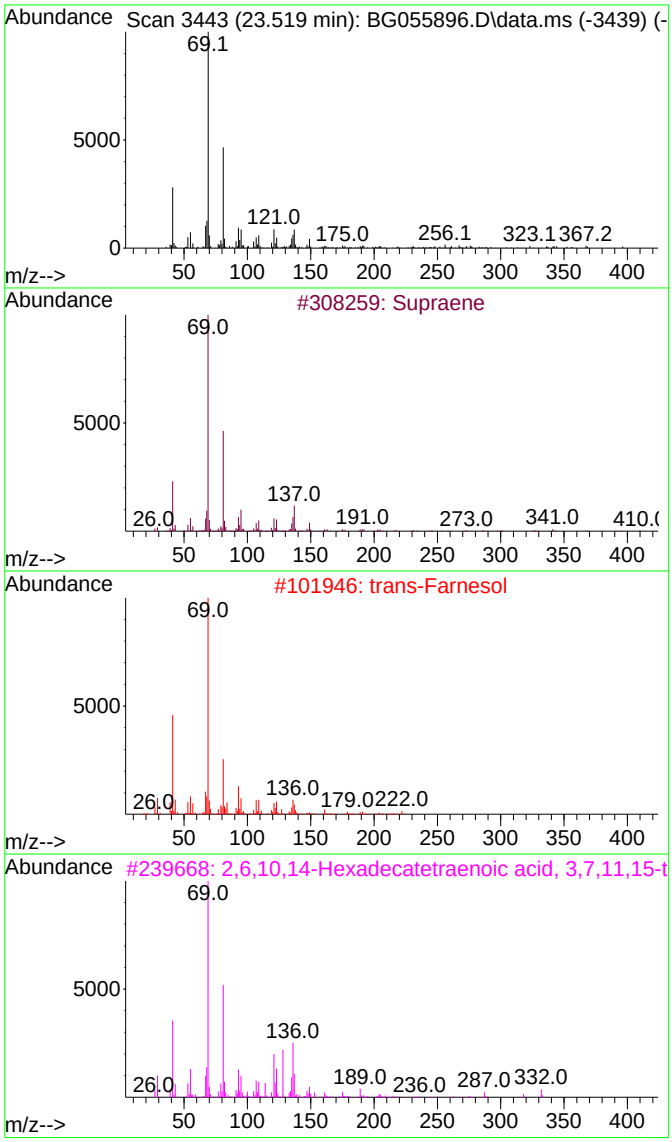
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

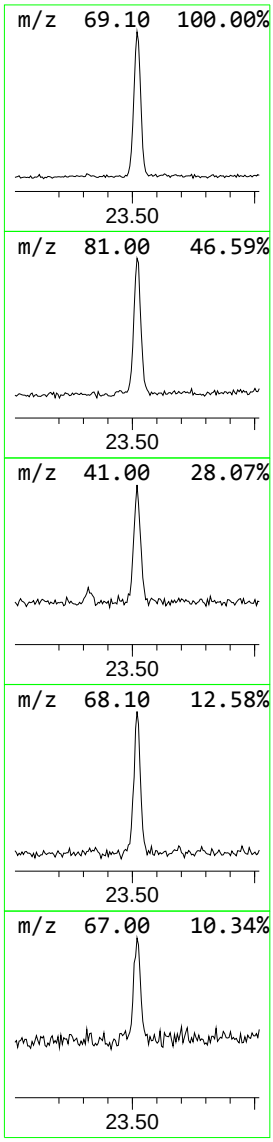
****

Peak Number 6 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.519	9.52 ng	253486	Perylene-d12	25.188

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	trans-Farnesol	222	C15H26O	000106-28-5	78
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4	5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	78
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055896.D
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.217	29.4	ng	409577	1	8.172	278973	20.0
n-Hexadecanoic ...	18.401	6.9	ng	220550	4	17.544	640830	20.0
9,10-Dimethylan...	19.312	2.2	ng	69669	4	17.544	640830	20.0
Octadecanoic acid	19.665	2.0	ng	65057	4	17.544	640830	20.0
11-Tricosene	21.433	2.7	ng	128073	5	21.827	949146	20.0
Supraene	23.519	9.5	ng	253486	6	25.188	532804	20.0