LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	326	334	339	rBV2	91087	141594	5.30%	1.023%
2	5.815	405	413	422	rBV	786685	1274995	47.75%	9.209%
3	7.448	683	691	699	rVB	864015	1487123	55.69%	10.742%
4	8.318	831	839	846	rBV2	144455	243650	9.12%	1.760%
5	9.522	1034	1044	1051	rBV	502307	928424	34.77%	6.706%
6	11.167	1314	1324	1331	rBV2	207160	356931	13.37%	2.578%
7	13.570	1725	1733	1740	rBV	1479731	2176363	81.50%	15.720%
8	13.776	1763	1768	1772	rVB4	17002	27012	1.01%	0.195%
9	14.945	1959	1967	1974	rBV2	289454	450244	16.86%	3.252%
10	16.438	2213	2221	2227	rBV2	1228145	1831813	68.60%	13.231%
11	17.701	2430	2436	2440	rBV2	360957	517657	19.39%	3.739%
12	17.742	2440	2443	2449	rVB	43975	61417	2.30%	0.444%
13	18.512	2568	2574	2580	rBV2	107103	159292	5.97%	1.151%
14	19.734	2777	2782	2785	rBV	78056	102976	3.86%	0.744%
15	19.769	2785	2788	2793	rVB6	37941	47554	1.78%	0.343%
16	20.098	2840	2844	2850	rVB2	63402	88821	3.33%	0.642%
17	20.274	2868	2874	2881	rBV	2192804	2670345	100.00%	19.288%
18	20.979	2989	2994	2997	rBV	187494	227399	8.52%	1.643%
19	21.555	3088	3092	3098	rVB6	49116	76151	2.85%	0.550%
20	22.019	3164	3171	3177	rBV2	235962	441229	16.52%	3.187%
21	22.842	3306	3311	3314	rVV7	19750	30932	1.16%	0.223%
22	23.206	3371	3373	3380	rVB7	20803	26845	1.01%	0.194%
23	24.428	3575	3581	3584	rBV8	24216	53057	1.99%	0.383%
24	25.586	3769	3778	3789	rVB4	134304	422696	15.83%	3.053%

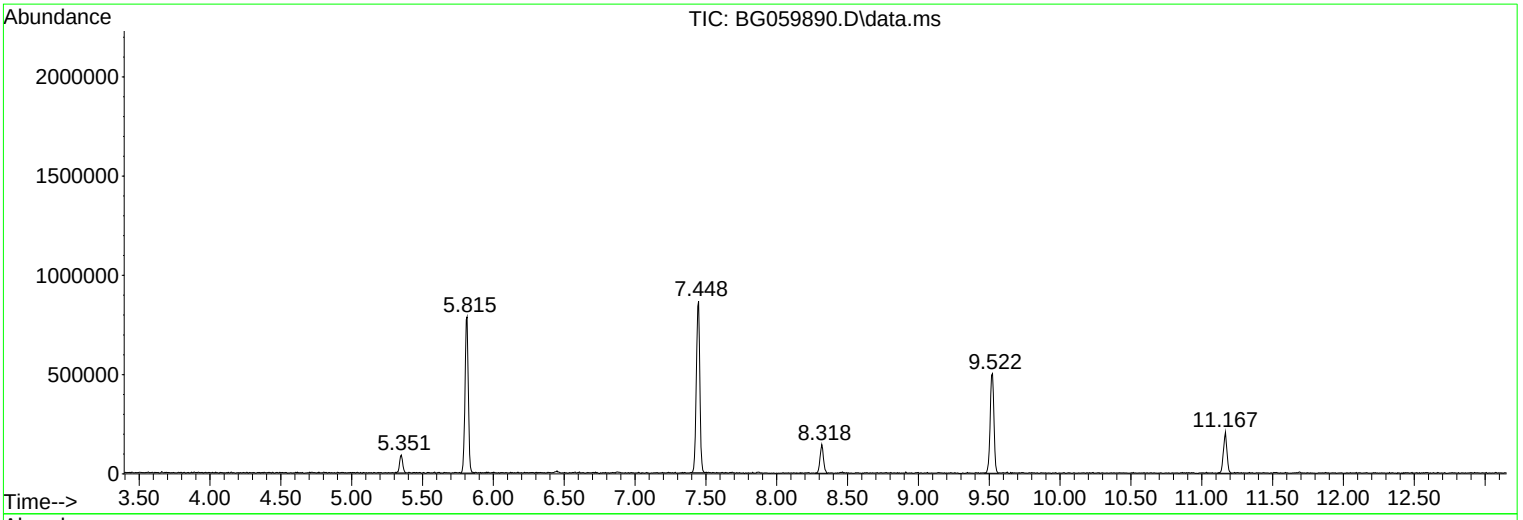
Sum of corrected areas: 13844520

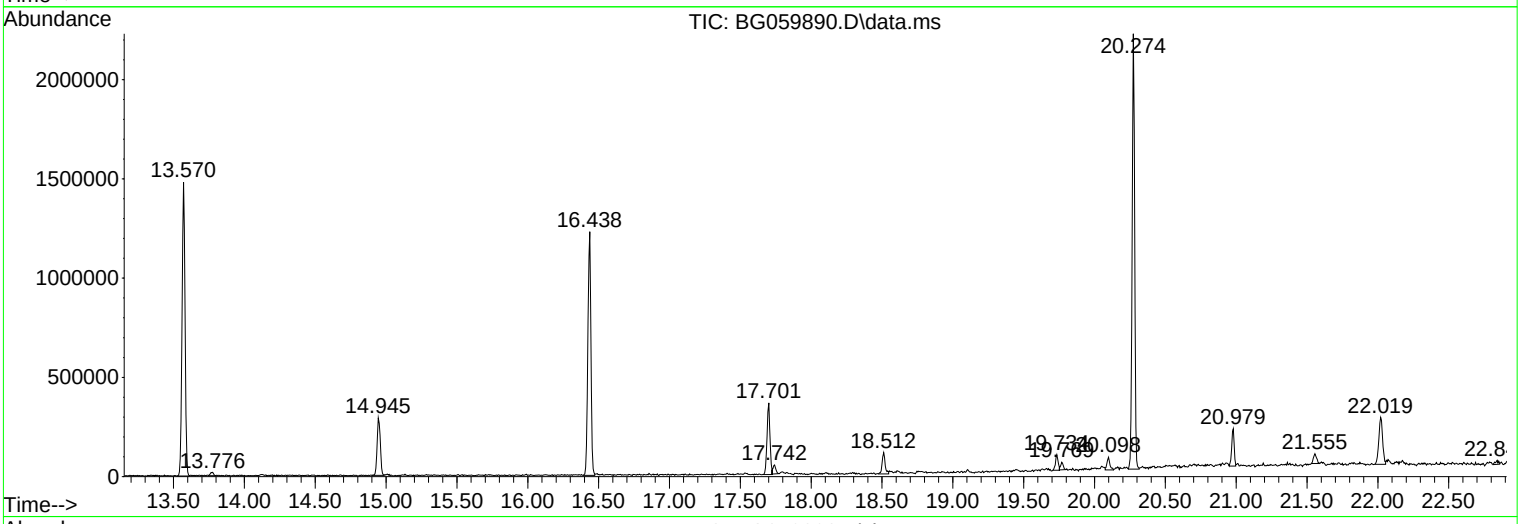
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

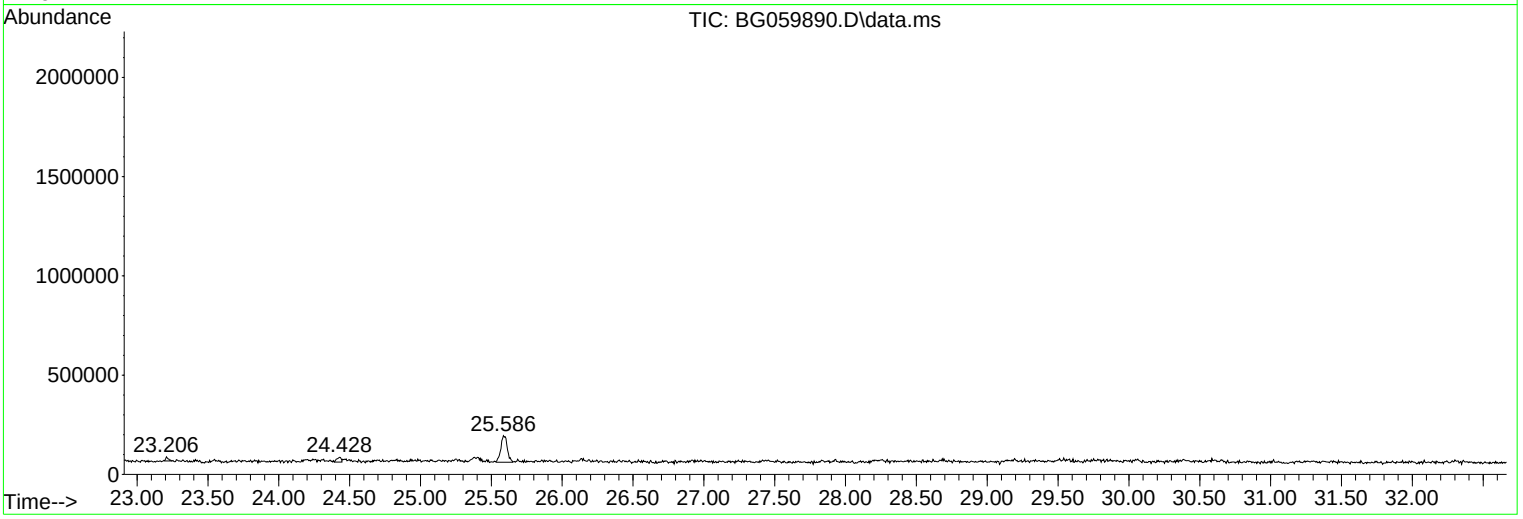
Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

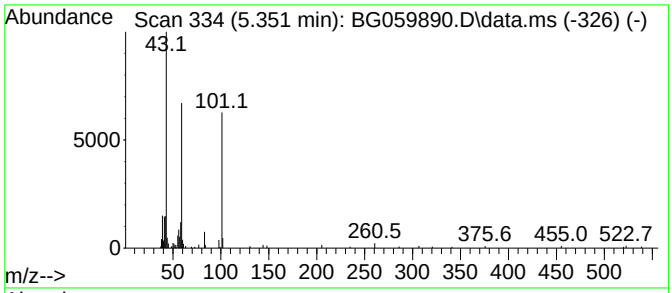
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

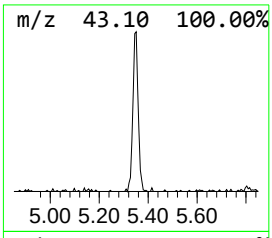
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

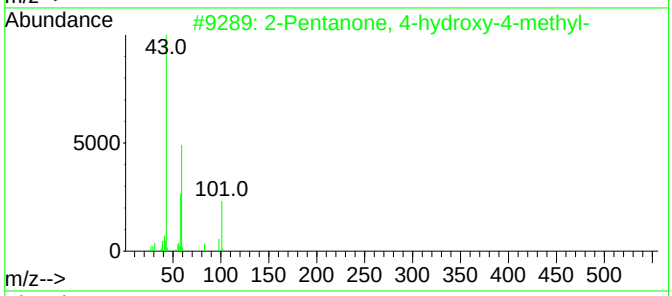
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

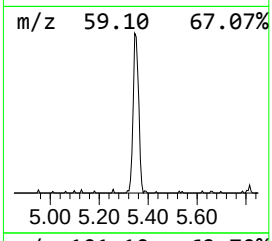
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.351	11.62 ng	141594	1,4-Dichlorobenzene-d4	8.318

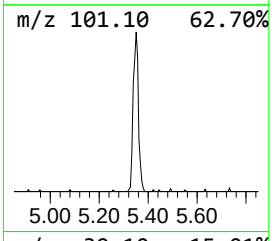
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	50
3	3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	39
4	Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O3	025333-21-5	39
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	35

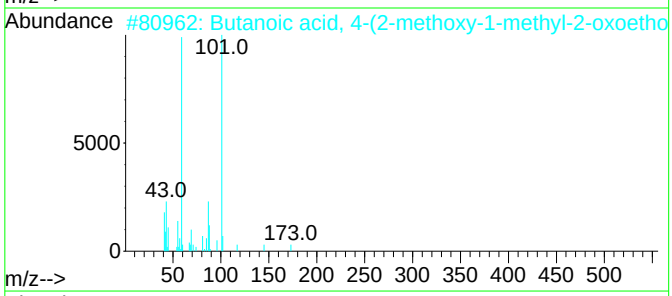


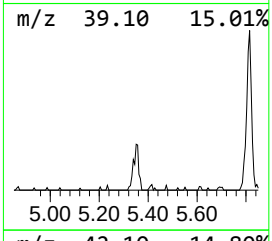


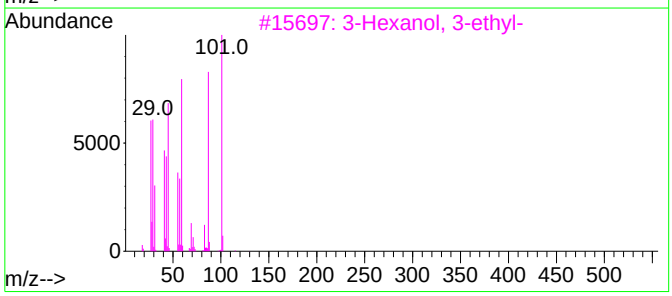


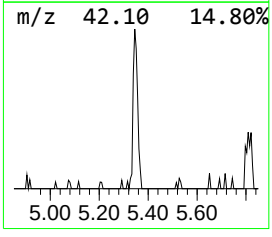












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

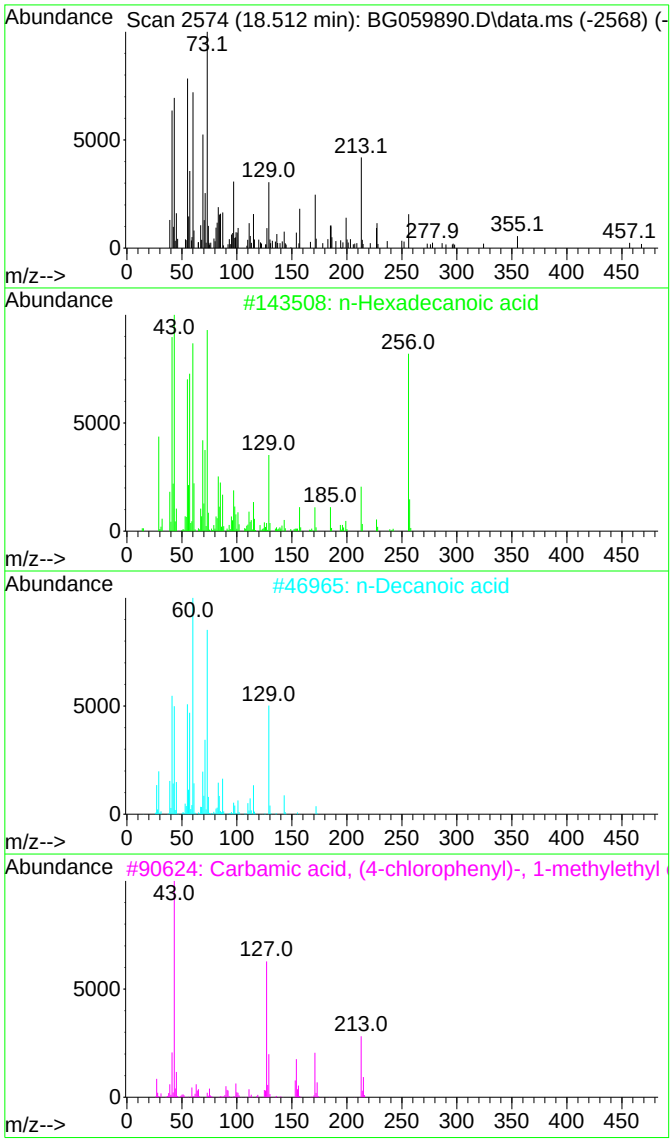
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

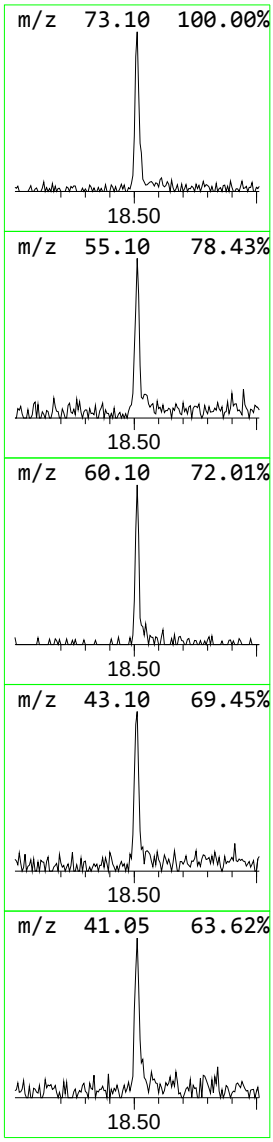
****

Peak Number 2 unknown18.512 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.512	6.15 ng	159292	Phenanthrene-d10	17.701

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	41
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Carbamic acid, (4-chlorophenyl)-...	213	C10H12ClNO2	002239-92-1	30
4	Dodecanoic acid	200	C12H24O2	000143-07-7	25
5	Undecanoic acid	186	C11H22O2	000112-37-8	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

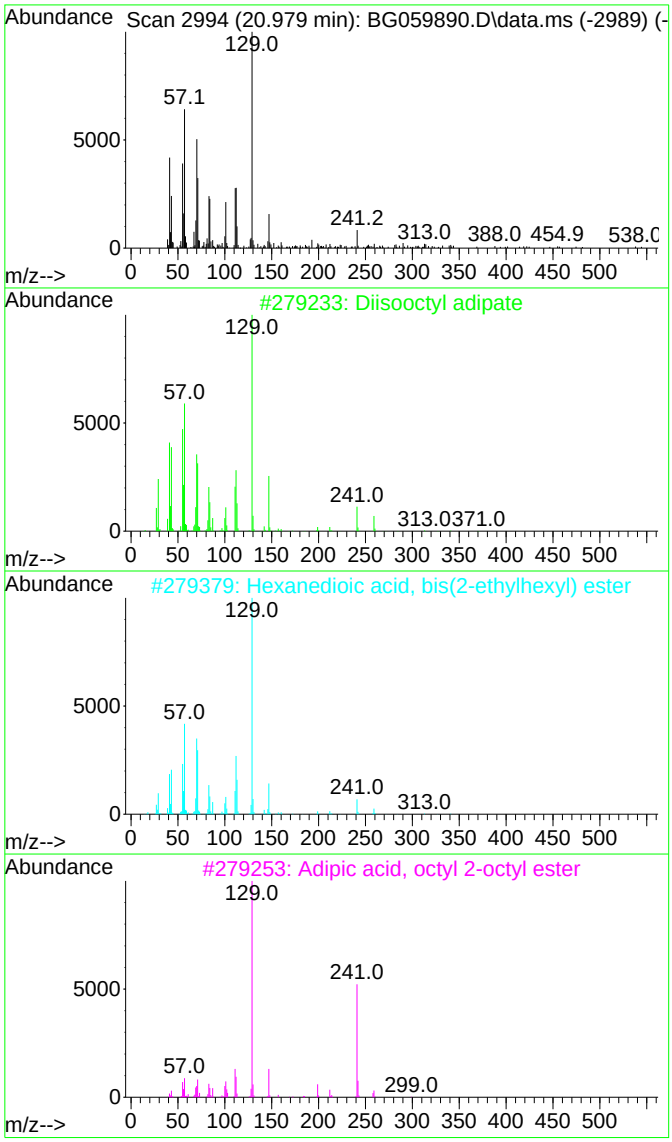
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

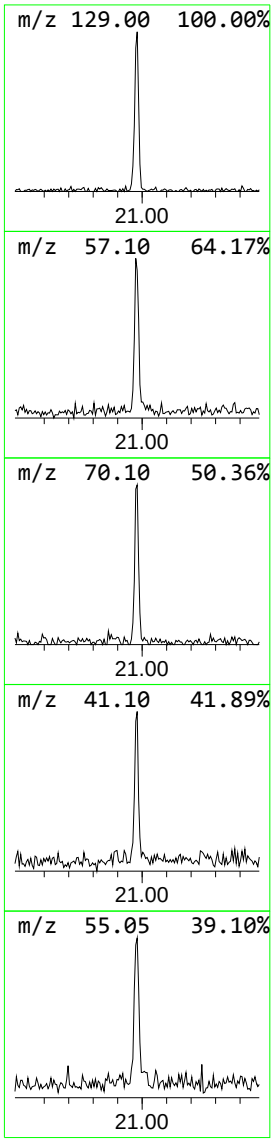
****

Peak Number 3 Diisooctyl adipate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.979	10.31 ng	227399	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	64
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	59
3	Adipic acid, octyl 2-octyl ester	370	C22H42O4	1000324-45-0	50
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	50
5	Succinic acid, ethyl 2-methylcyc...	242	C13H22O4	1000329-81-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

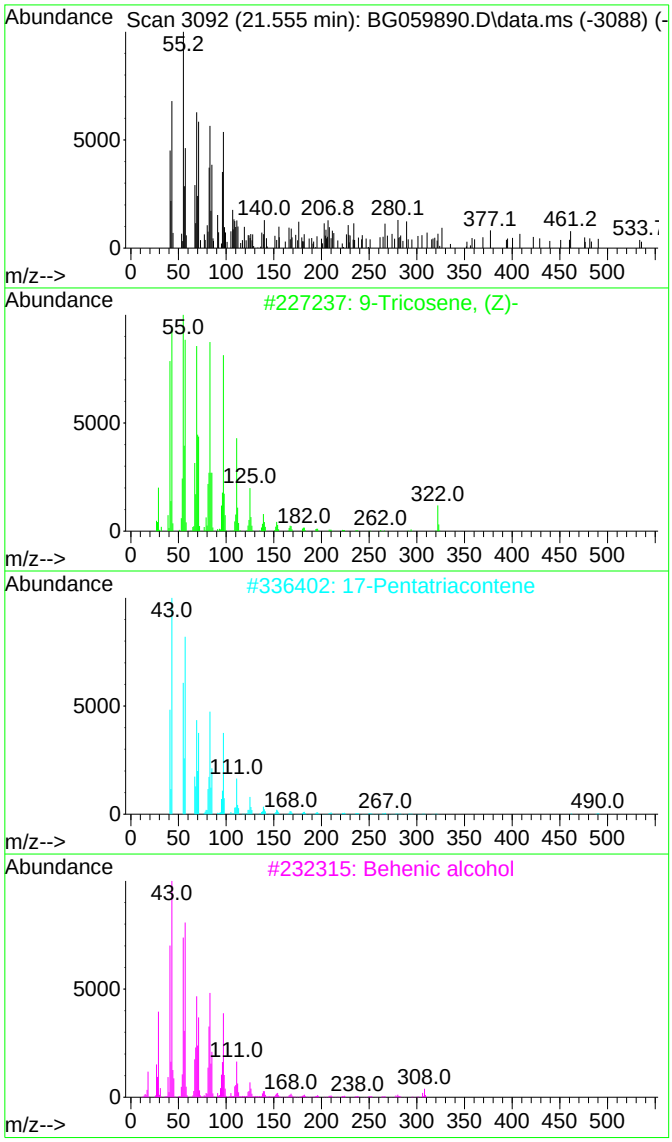
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

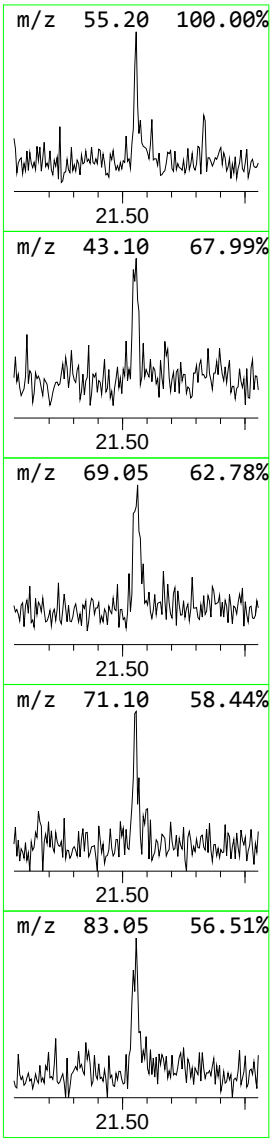
****

Peak Number 4 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	3.45 ng	76151	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	51
2	17-Pentatriacontene	491	C35H70	006971-40-0	43
3	Behenic alcohol	326	C22H46O	000661-19-8	43
4	11-Tricosene	322	C23H46	052078-56-5	43
5	2-Methyl-2-docosene	322	C23H46	1000131-16-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

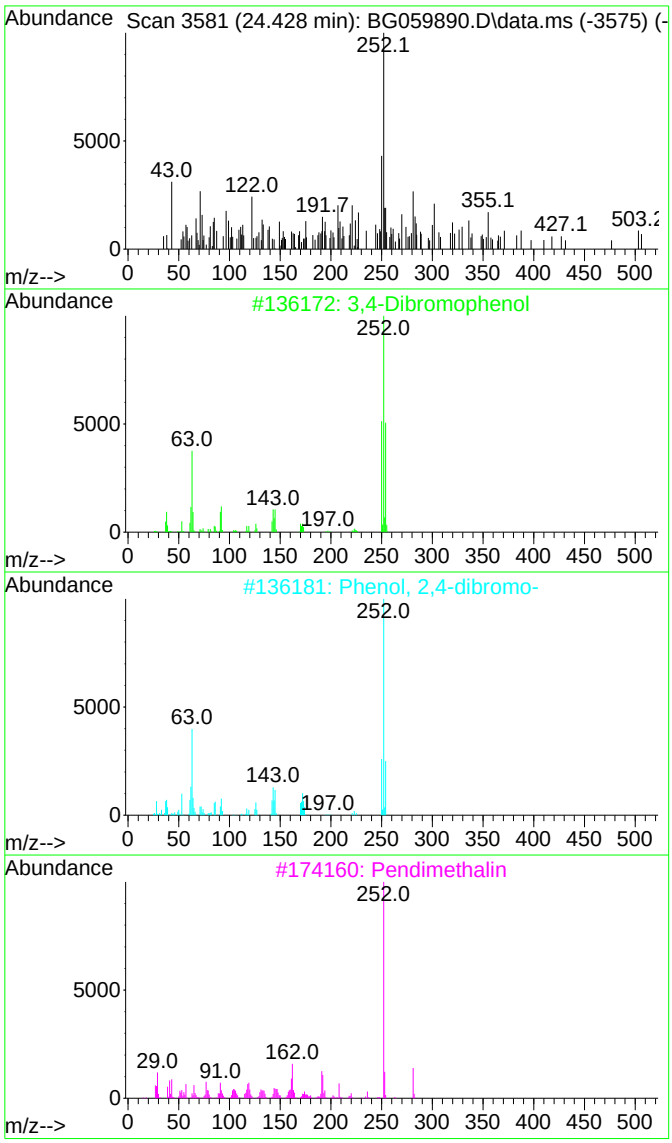
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

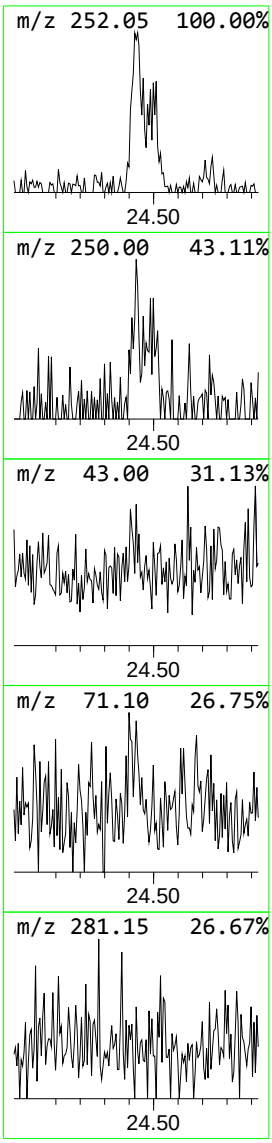
****

Peak Number 5 unknown24.428 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.428	2.51 ng	53057	Perylene-d12	25.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dibromophenol	250	C6H4Br2O	1010487-11-5	46
2	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	43
3	Pendimethalin	281	C13H19N3O4	040487-42-1	38
4	6-Ethylthiopurine, TMS	252	C10H16N4SSi	1000497-86-9	38
5	2-(4-Chlorophenyl)-1H-indole-3-c...	252	C15H9ClN2	1000482-53-3	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059890.D
Acq On : 25 Nov 2023 13:58
Operator : MA/JU
Sample : 05470-01
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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-...	5.351	11.6	ng	141594	1	8.318	243650	20.0
unknown18.512	18.512	6.2	ng	159292	4	17.701	517657	20.0
Diisooctyl adipate	20.979	10.3	ng	227399	5	22.019	441229	20.0
9-Tricosene, (Z)-	21.555	3.5	ng	76151	5	22.019	441229	20.0
unknown24.428	24.428	2.5	ng	53057	6	25.598	422696	20.0