LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

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-BG042024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.525	423	432	441	rBV	450262	685081	24.82%	6.831%
2	7.112	694	702	711	rVB	452803	764557	27.70%	7.624%
3	7.934	835	842	849	rVB	85236	138357	5.01%	1.380%
4	9.092	1030	1039	1048	rBV	291872	505871	18.33%	5.044%
5	10.737	1311	1319	1326	rVB	103534	182752	6.62%	1.822%
6	13.193	1730	1737	1745	rBV	869514	1287365	46.64%	12.837%
7	14.568	1964	1971	1977	rBV	194074	301850	10.94%	3.010%
8	16.060	2218	2225	2234	rBV	990901	1445163	52.36%	14.411%
9	16.683	2325	2331	2338	rVB	14059	36222	1.31%	0.361%
10	17.317	2432	2439	2447	rBV	305952	451159	16.35%	4.499%
11	18.210	2587	2591	2597	rBV3	52085	73906	2.68%	0.737%
12	18.481	2629	2637	2641	rVV2	88960	188034	6.81%	1.875%
13	18.522	2641	2644	2650	rVB5	39924	71068	2.57%	0.709%
14	19.485	2805	2808	2813	rBV4	23297	30322	1.10%	0.302%
15	19.938	2879	2885	2894	rBV	2193976	2759940	100.00%	27.521%
16	21.248	3105	3108	3115	rVB3	28370	40859	1.48%	0.407%
17	21.577	3158	3164	3170	rBV2	319988	510053	18.48%	5.086%
18	21.789	3196	3200	3205	rVB3	34712	51567	1.87%	0.514%
19	24.697	3688	3695	3704	rVB	193078	504294	18.27%	5.029%

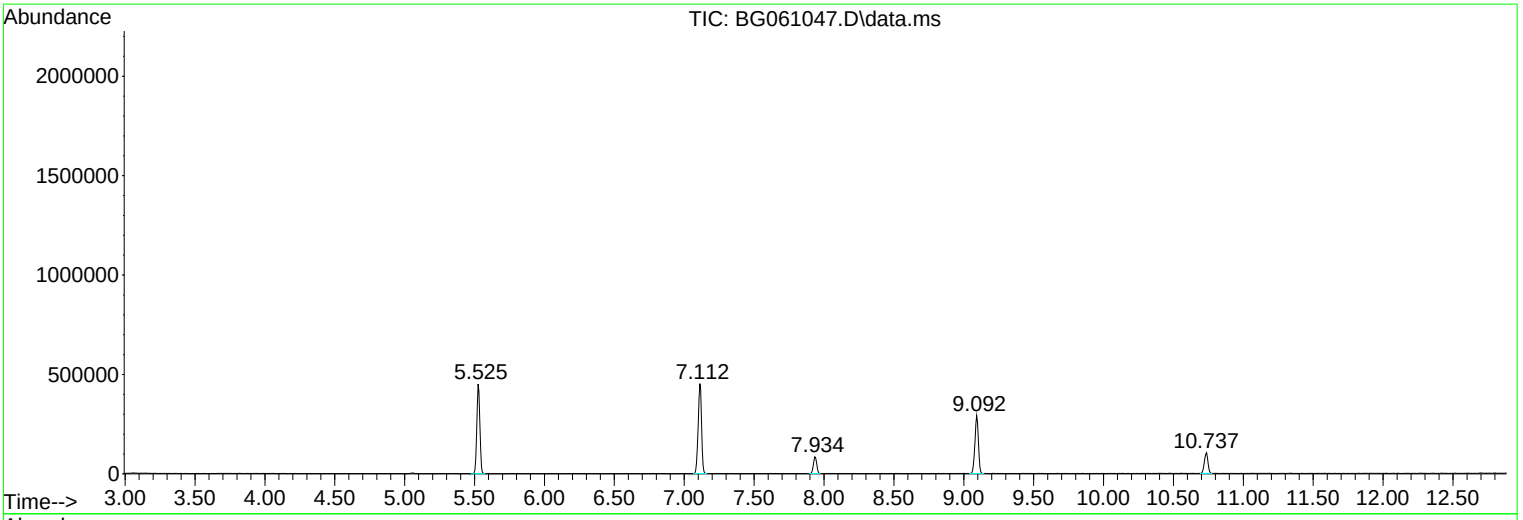
Sum of corrected areas: 10028420

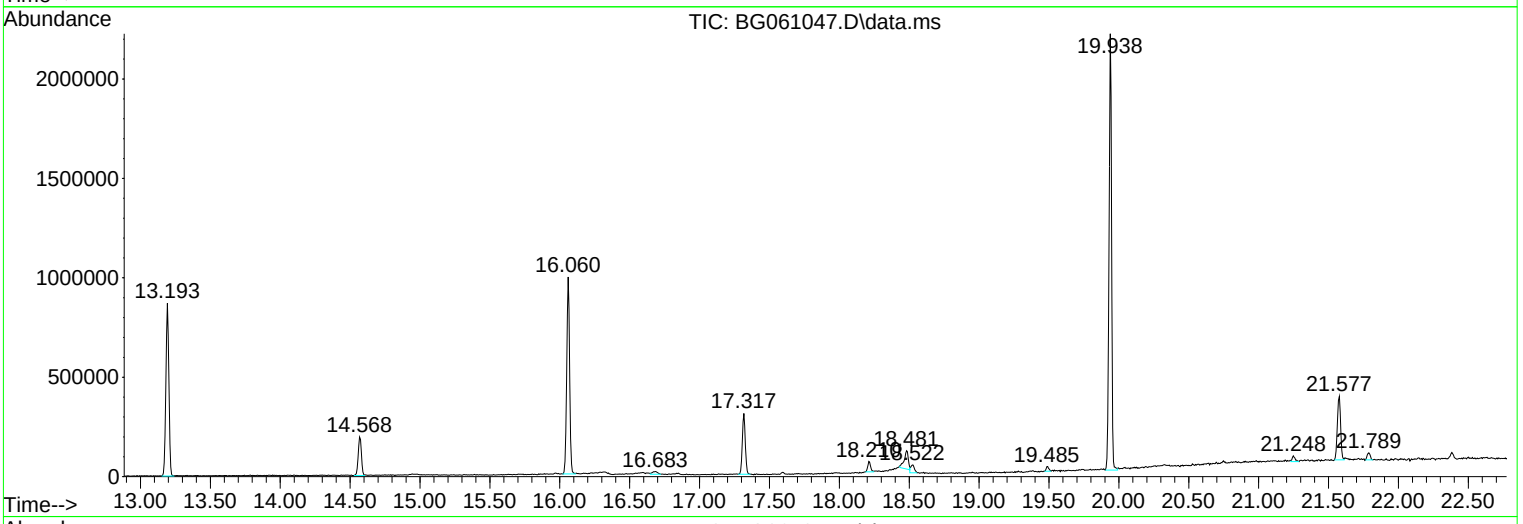
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

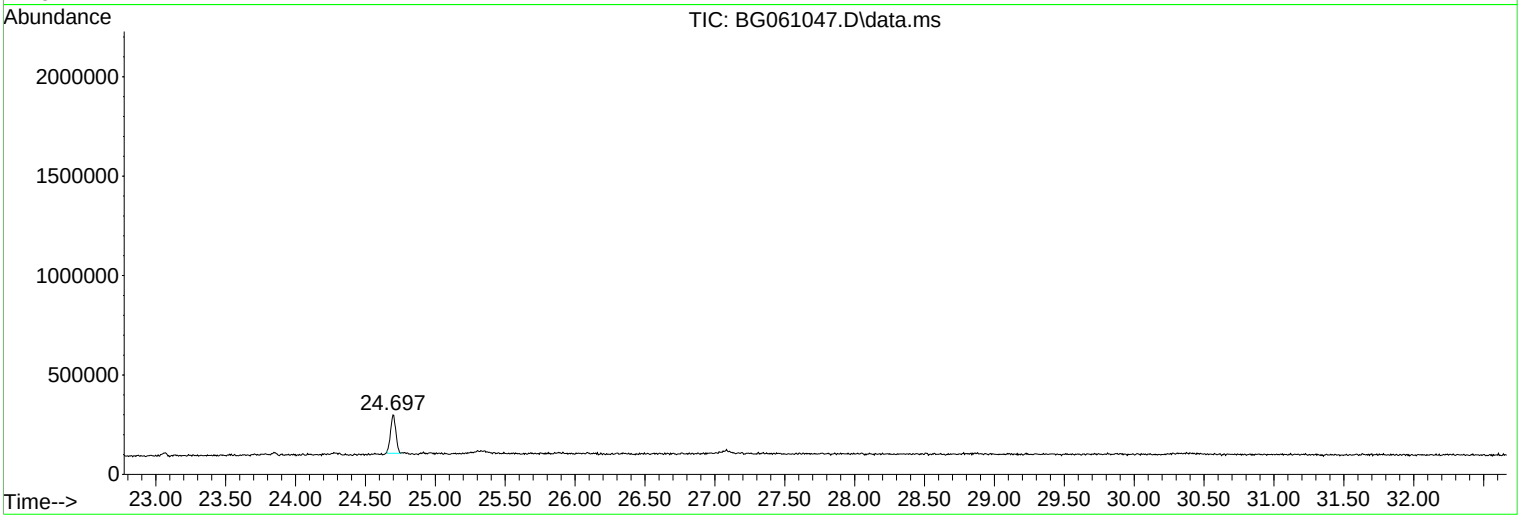
Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.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\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

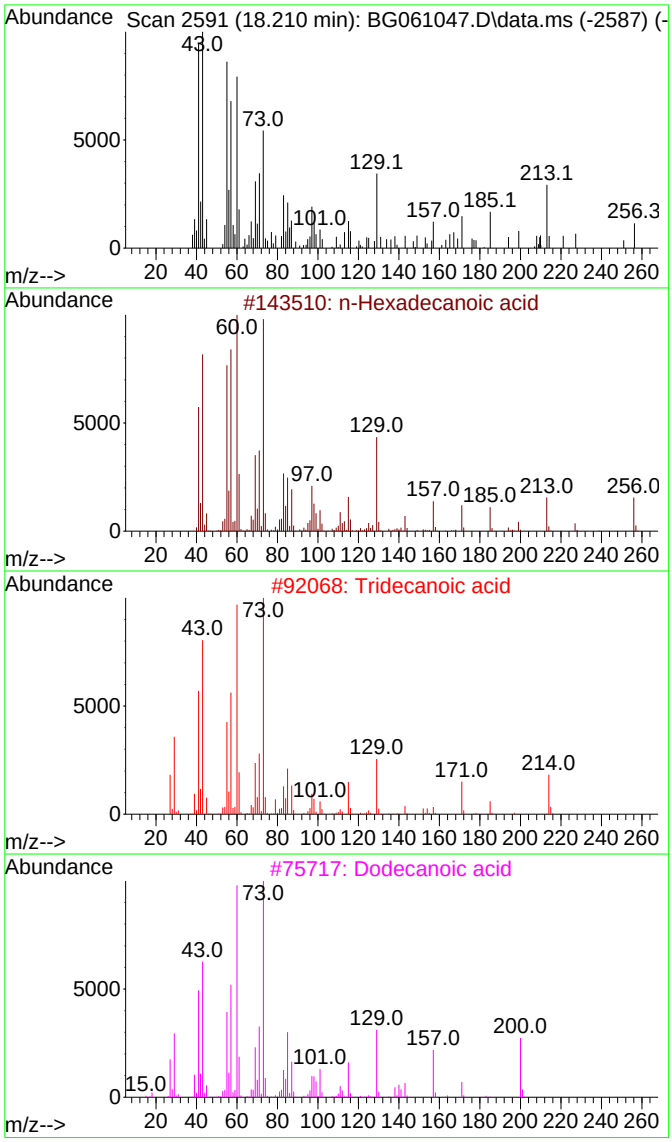
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

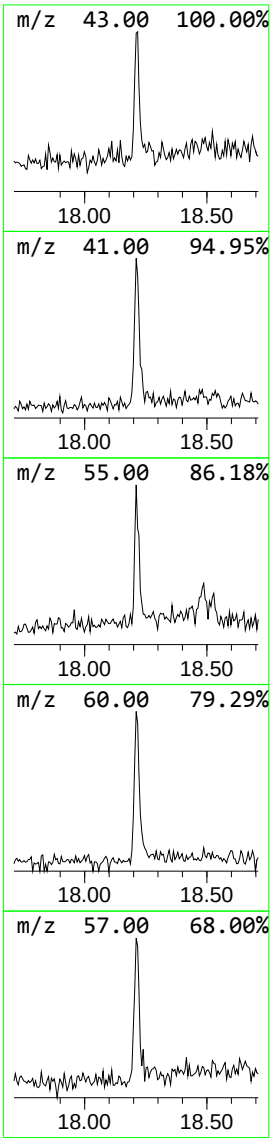
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	3.28 ng	73906	Phenanthrene-d10	17.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Dodecanoic acid	200	C12H24O2	000143-07-7	47
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

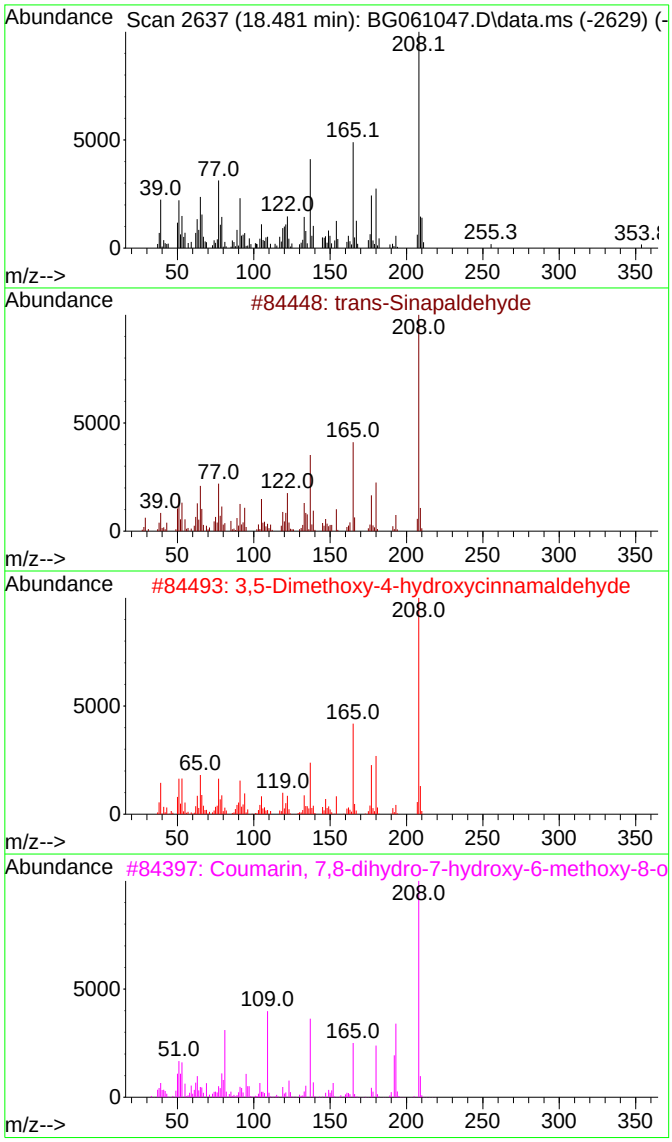
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

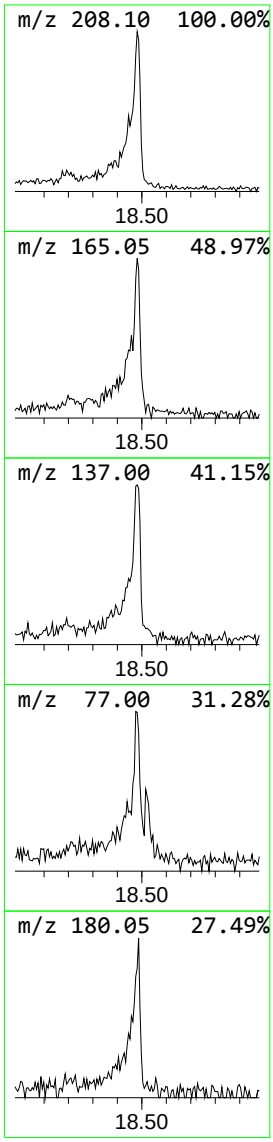
****

Peak Number 2 trans-Sinapaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.481	8.34 ng	188034	Phenanthrene-d10	17.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	93
2	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	90
3	Coumarin, 7,8-dihydro-7-hydroxy-...	208	C10H8O5	1000263-13-6	58
4	2H-1-Benzopyran-2-one, 7,8-dihyd...	208	C10H8O5	000574-84-5	52
5	Benzo[c]cinnoline, 4,7-dimethyl-	208	C14H12N2	020684-54-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

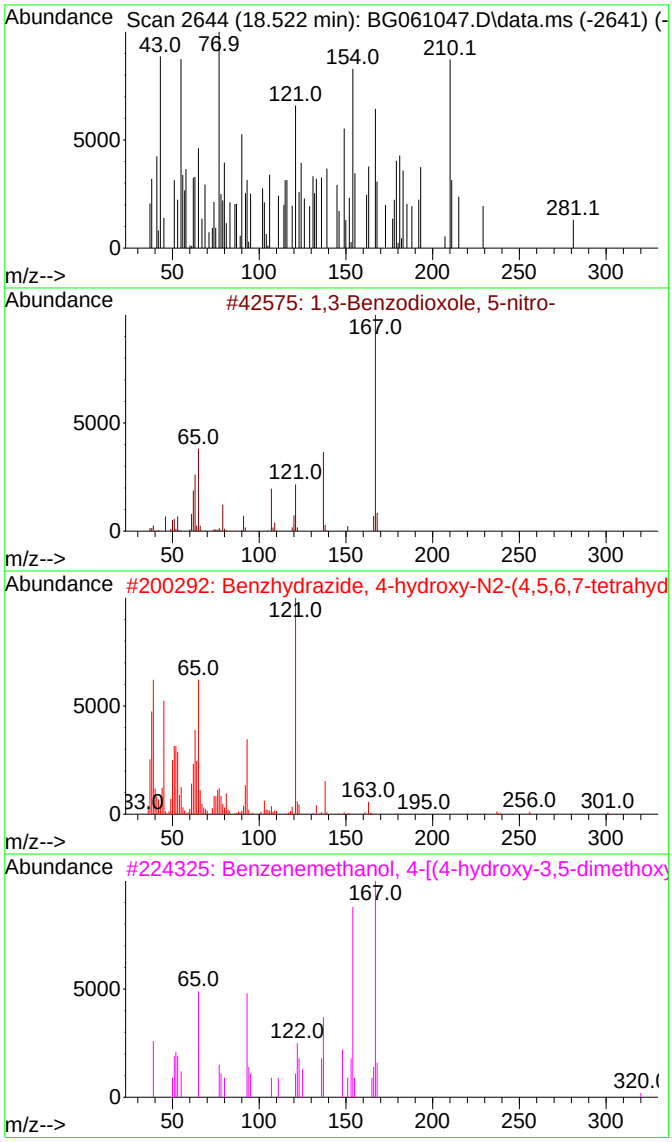
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

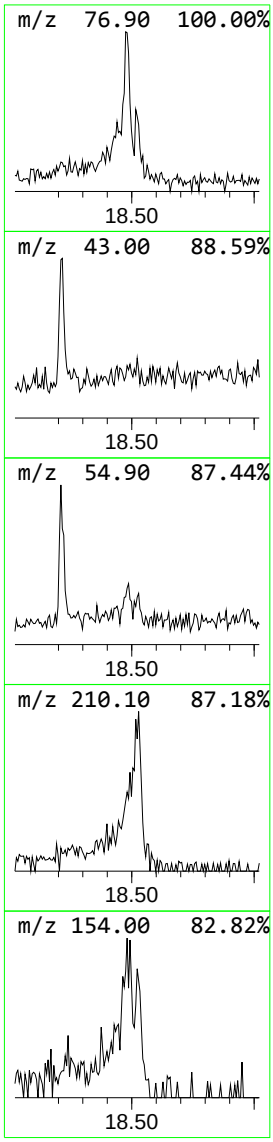
****

Peak Number 3 unknown18.522 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.522	3.15 ng	71068	Phenanthrene-d10	17.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzodioxole, 5-nitro-	167	C7H5NO4	002620-44-2	27
2	Benzhydrazide, 4-hydroxy-N2-(4,5...	301	C13H11N5O4	1010294-58-5	27
3	Benzenemethanol, 4-[(4-hydroxy-3...	320	C17H20O6	055525-43-4	23
4	2,3,5,7,13,14-Hexaazatetracyclo[...	210	C10H6N6	1000388-86-0	14
5	Urea, N,N'-bis(4-nitrophenyl)-	302	C13H10N4O5	000587-90-6	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

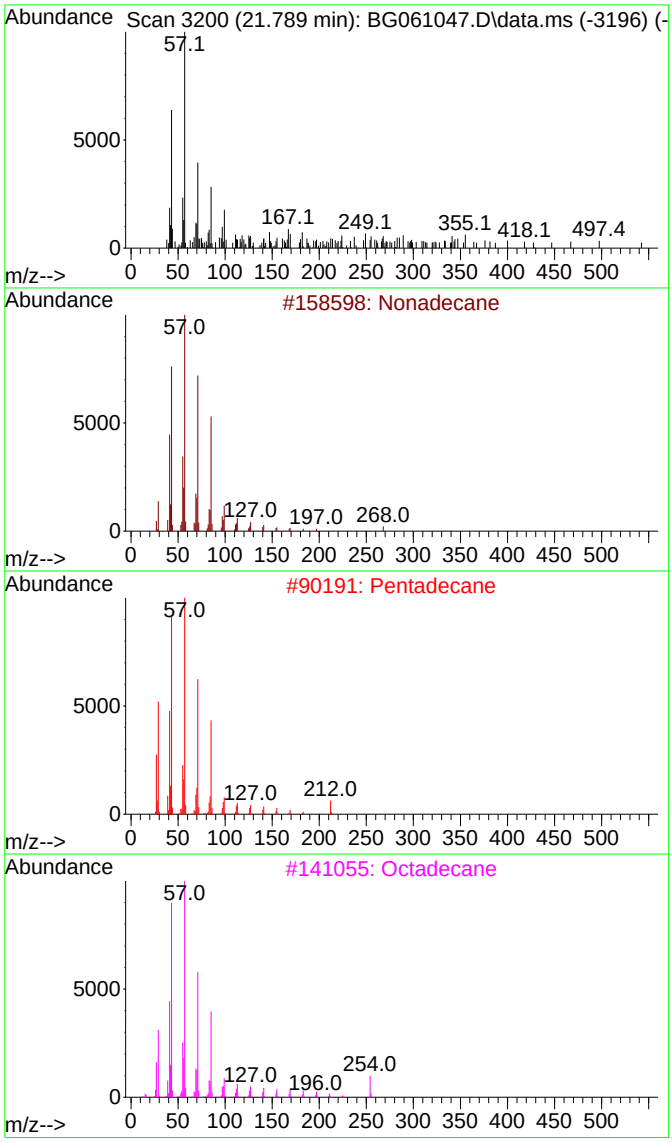
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

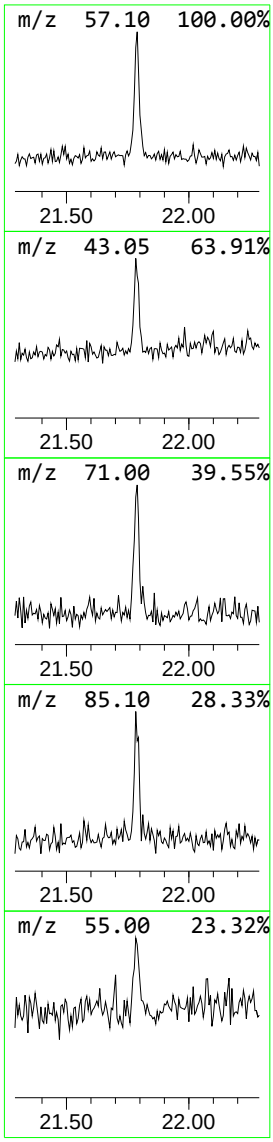
****

Peak Number 4 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.789	2.02 ng	51567	Chrysene-d12	21.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	70
2	Pentadecane	212	C15H32	000629-62-9	70
3	Octadecane	254	C18H38	000593-45-3	70
4	Heneicosane	296	C21H44	000629-94-7	62
5	Decane	142	C10H22	000124-18-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042924\
Data File : BG061047.D
Acq On : 29 Apr 2024 14:47
Operator : MA/JU
Sample : PB160581BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160581BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.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
n-Hexadecanoic ...	18.210	3.3	ng	73906	4	17.317	451159	20.0
trans-Sinapalde...	18.481	8.3	ng	188034	4	17.317	451159	20.0
unknown18.522	18.522	3.1	ng	71068	4	17.317	451159	20.0
Nonadecane	21.789	2.0	ng	51567	5	21.577	510053	20.0