LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.336	155	161	166	rBV2	9831	20827	1.12%	0.173%
2	5.164	295	302	311	rBV2	14618	28451	1.52%	0.236%
3	5.640	376	383	393	rBV	615898	1036037	55.48%	8.589%
4	7.238	648	655	673	rBV	648146	1174916	62.91%	9.740%
5	8.066	789	796	803	rBV	145545	251074	13.44%	2.081%
6	9.235	987	995	1005	rBV	402609	754891	40.42%	6.258%
7	9.458	1025	1033	1040	rBV	32952	58813	3.15%	0.488%
8	10.880	1268	1275	1284	rBV	198689	366523	19.63%	3.038%
9	13.318	1682	1690	1697	rBV	1032502	1589077	85.09%	13.173%
10	14.140	1822	1830	1837	rBV2	16042	29124	1.56%	0.241%
11	14.698	1919	1925	1934	rVB	312917	492795	26.39%	4.085%
12	16.184	2172	2178	2186	rBV	749496	1153967	61.79%	9.566%
13	16.819	2283	2286	2295	rBV3	16747	29343	1.57%	0.243%
14	17.036	2318	2323	2332	rVB	22726	39579	2.12%	0.328%
15	17.330	2369	2373	2379	rBV6	9288	20523	1.10%	0.170%
16	17.442	2386	2392	2399	rBV	347126	528403	28.29%	4.380%
17	17.500	2399	2402	2408	rVB3	14217	21191	1.13%	0.176%
18	18.223	2520	2525	2530	rBV3	14686	25870	1.39%	0.214%
19	18.323	2536	2542	2551	rBV2	96597	177048	9.48%	1.468%
20	19.175	2683	2687	2693	rBV3	21407	27599	1.48%	0.229%
21	19.592	2755	2758	2768	rBV5	30706	54959	2.94%	0.456%
22	19.715	2776	2779	2785	rVB2	17885	28507	1.53%	0.236%
23	20.044	2830	2835	2845	rVB	1449869	1867560	100.00%	15.482%
24	20.608	2928	2931	2937	rVB5	36433	46921	2.51%	0.389%
25	20.725	2948	2951	2954	rBV	33912	41141	2.20%	0.341%
26	21.342	3052	3056	3062	rBV	91435	146894	7.87%	1.218%
27	21.589	3094	3098	3104	rVB	171851	241642	12.94%	2.003%
28	21.724	3115	3121	3130	rVB2	308306	570690	30.56%	4.731%
29	22.000	3164	3168	3173	rBV	58246	84249	4.51%	0.698%
30	24.021	3508	3512	3517	rVB3	54283	105392	5.64%	0.874%
31	24.990	3670	3677	3691	rVB2	182974	545314	29.20%	4.521%
32	31.752	4816	4828	4844	rBV	105396	503648	26.97%	4.175%

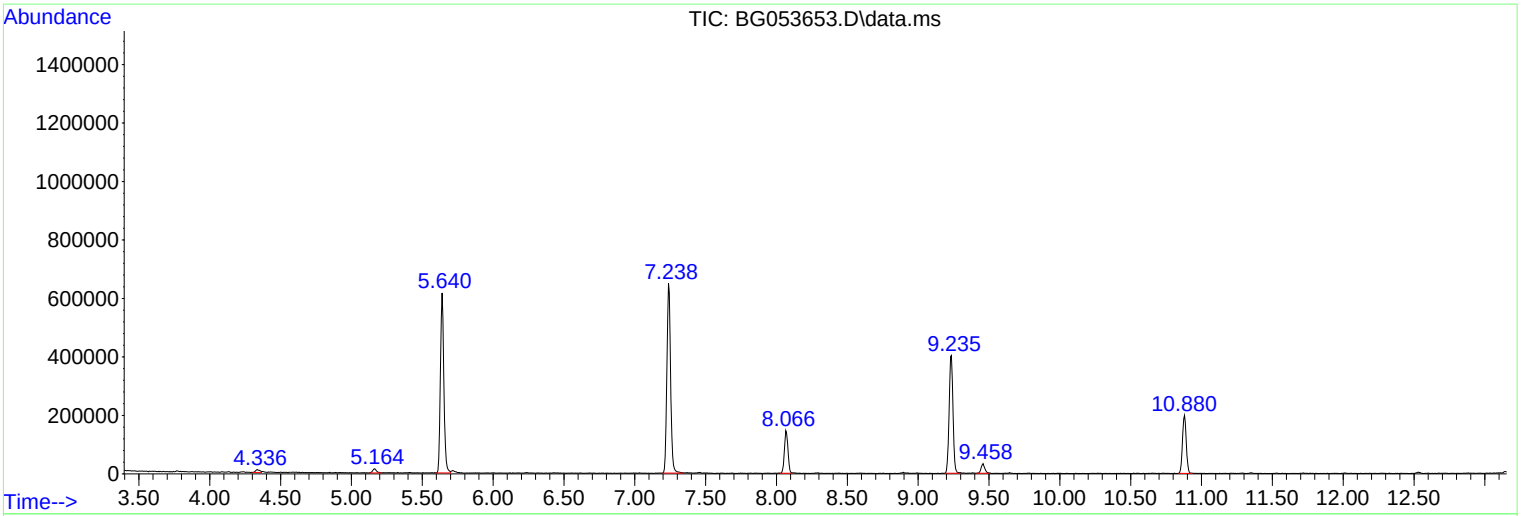
Sum of corrected areas: 12062968

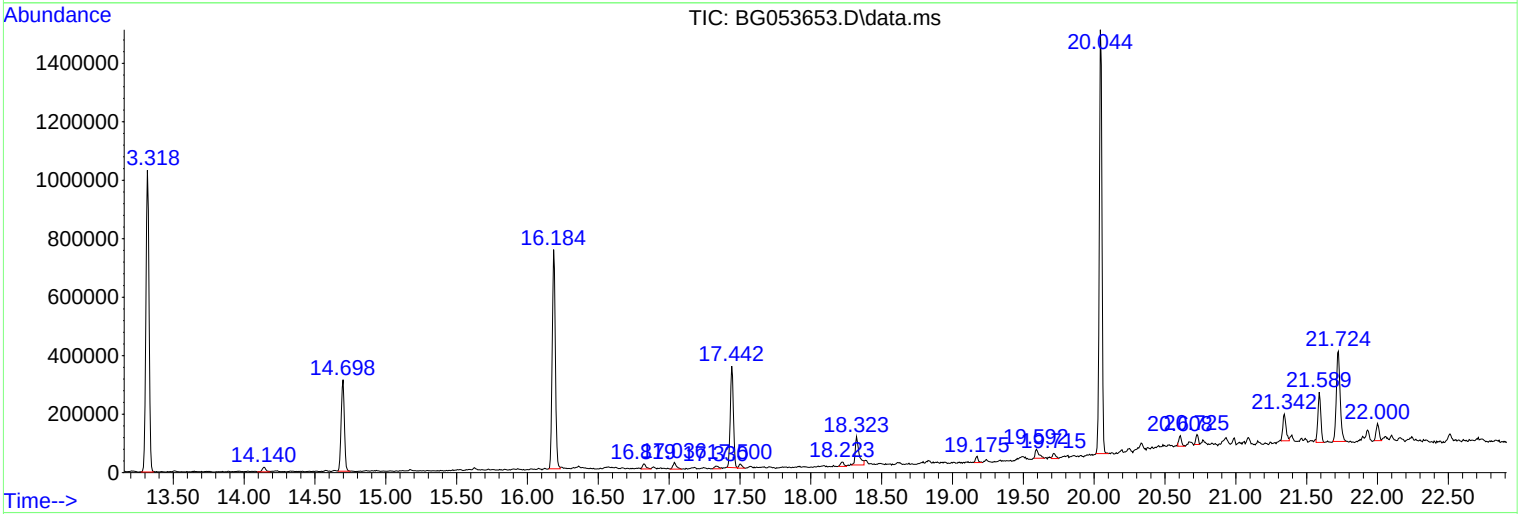
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

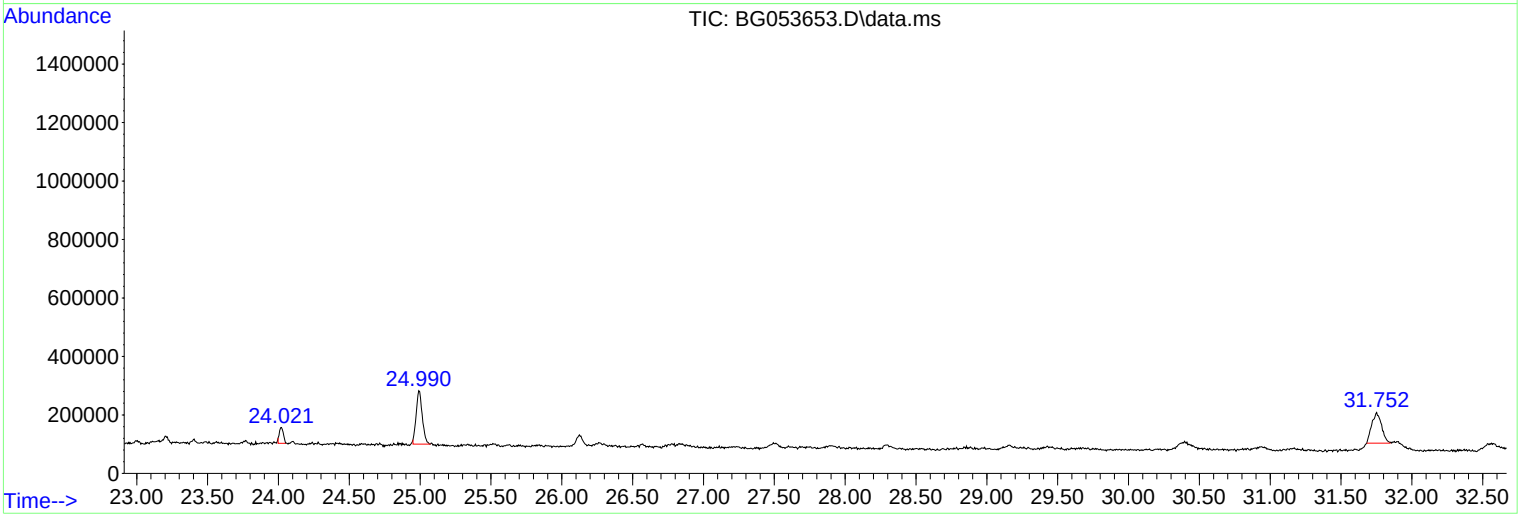
Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

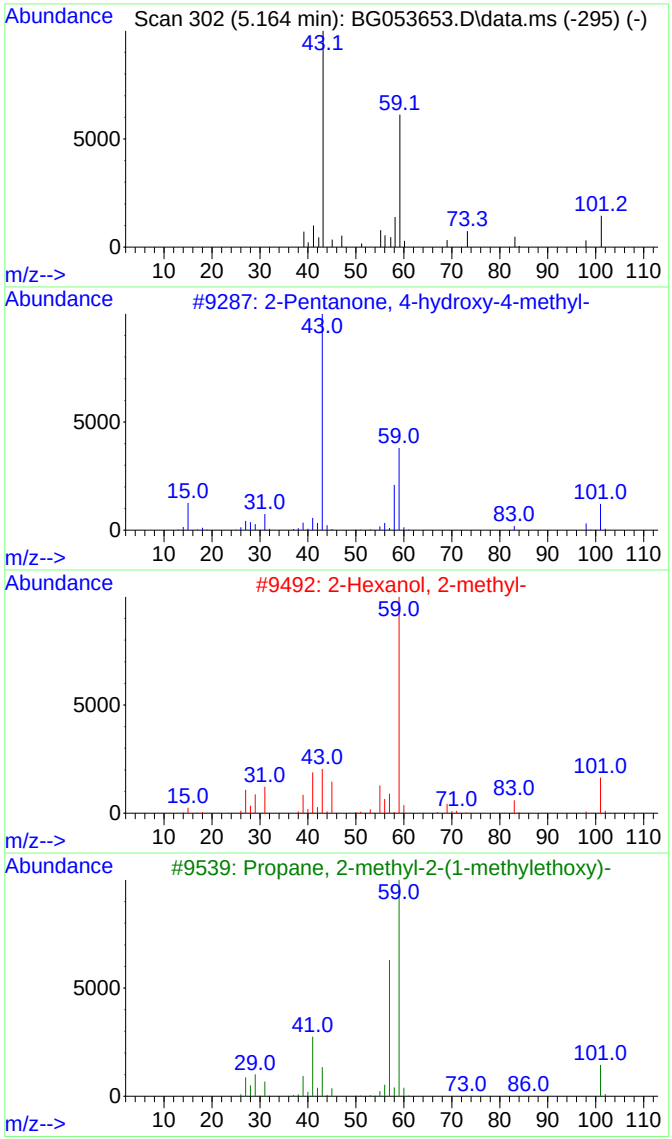
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

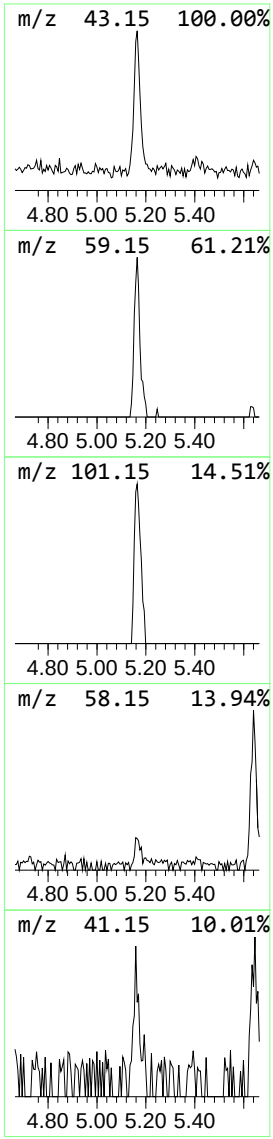
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.164	2.27 ng	28451	1,4-Dichlorobenzene-d4	8.066

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	37
4	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	33
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

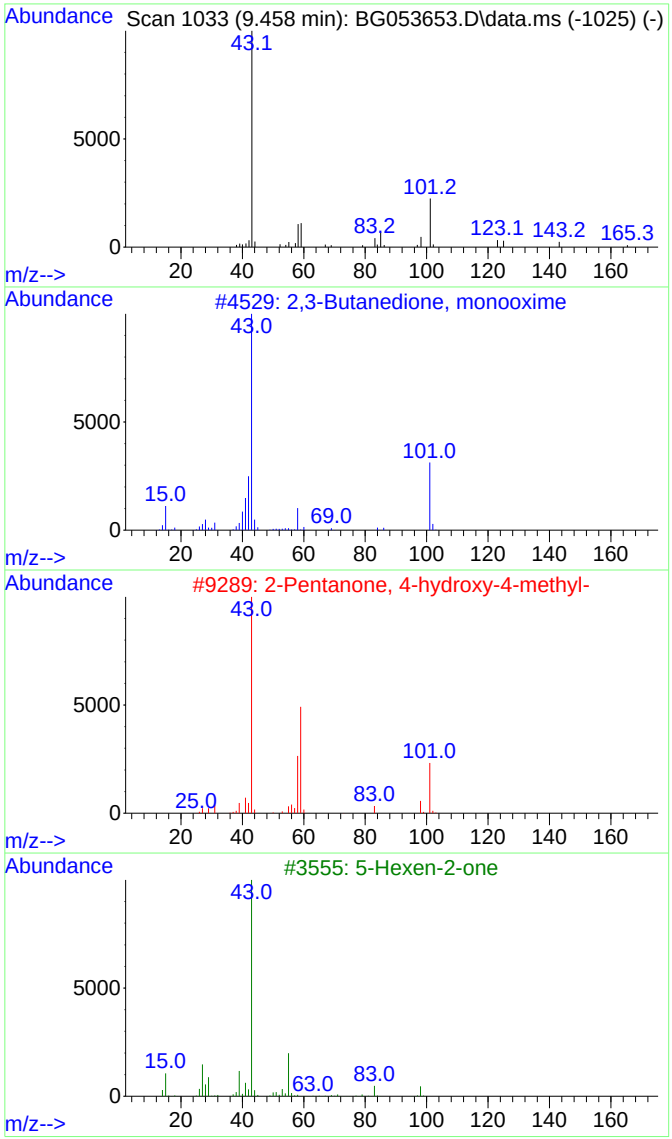
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

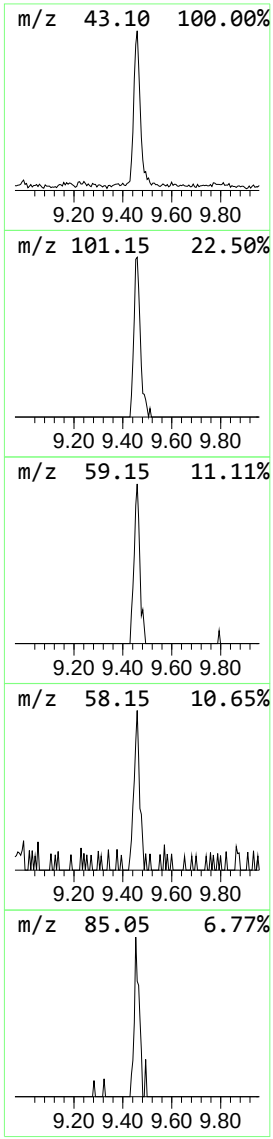
****

Peak Number 2 unknown9.458 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	4.68 ng	58813	1,4-Dichlorobenzene-d4	8.066

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	1,4-Dimethyl-5-oxabicyclo[2.1.0]...	98	C6H10O	002316-03-2	9
5	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

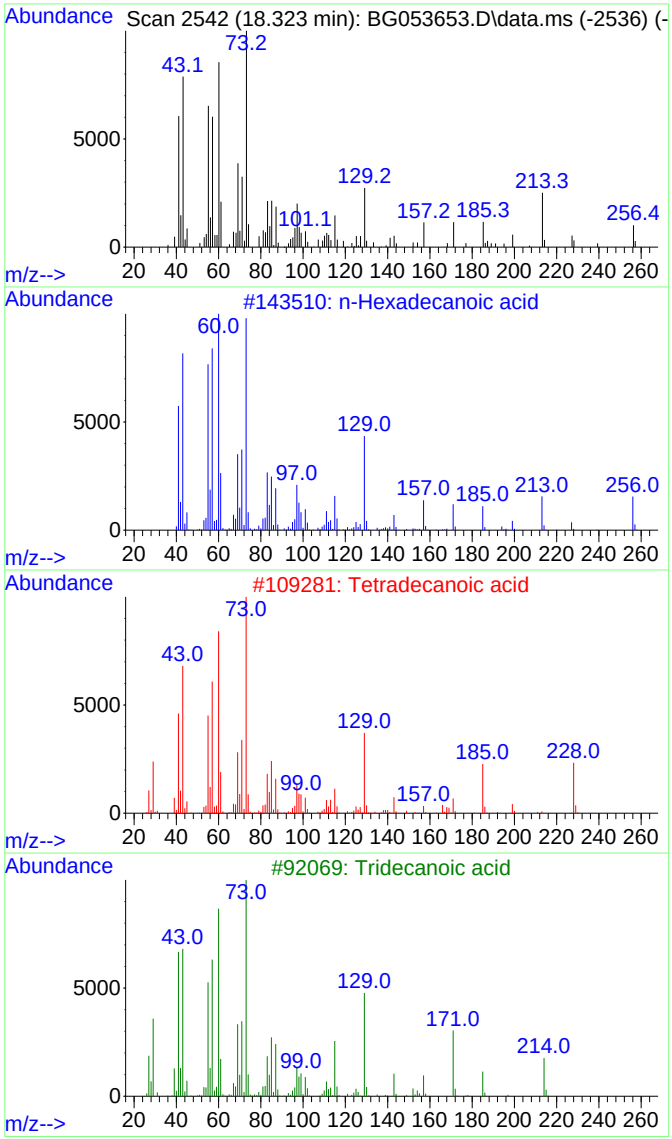
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

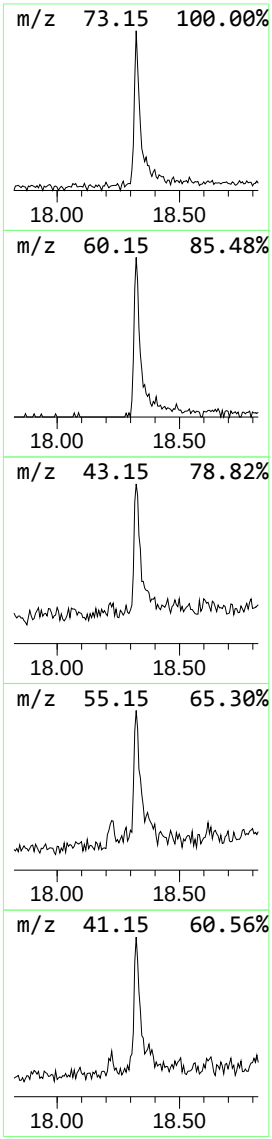
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.323	6.70 ng	177048	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

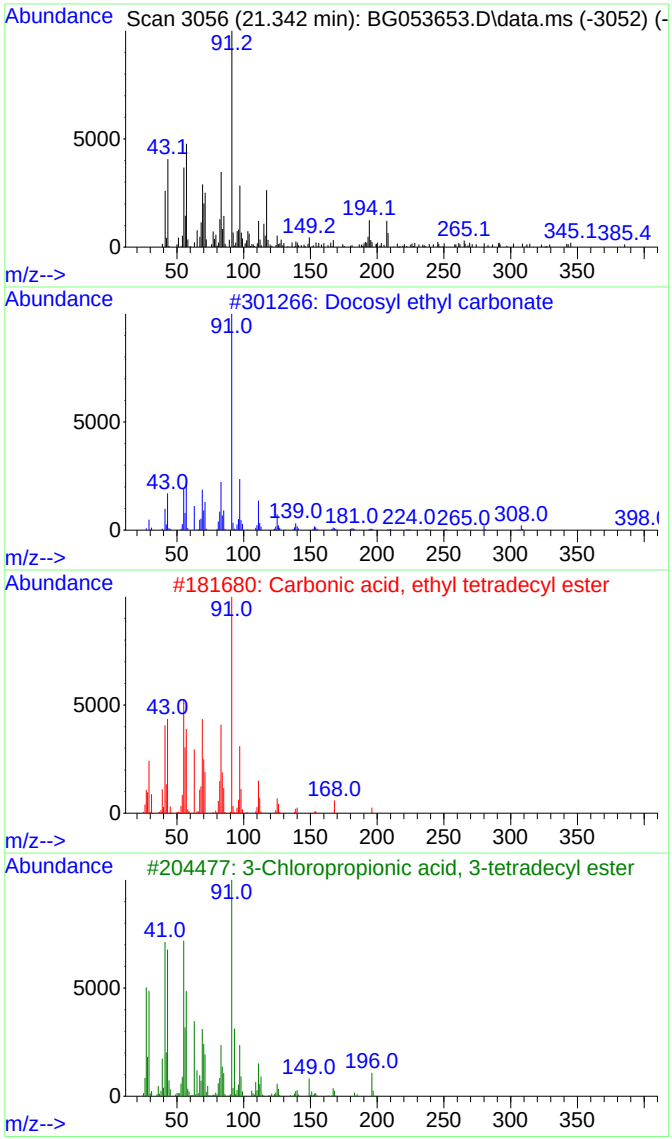
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

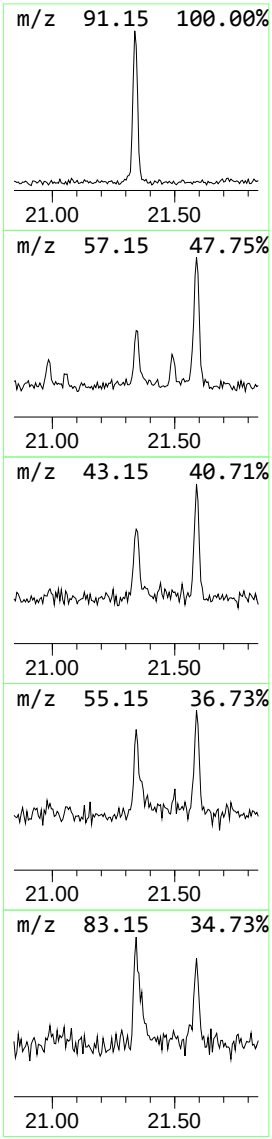
****

Peak Number 4 unknown21.342 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.342	5.15 ng	146894	Chrysene-d12	21.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl ethyl carbonate	398	C25H50O3	1000373-79-2	47
2	Carbonic acid, ethyl tetradecyl ...	286	C17H34O3	1000314-59-4	38
3	3-Chloropropionic acid, 3-tetrad...	304	C17H33ClO2	1010282-04-1	22
4	Cyclobutanecarboxylic acid, benz...	190	C12H14O2	199593-03-8	22
5	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

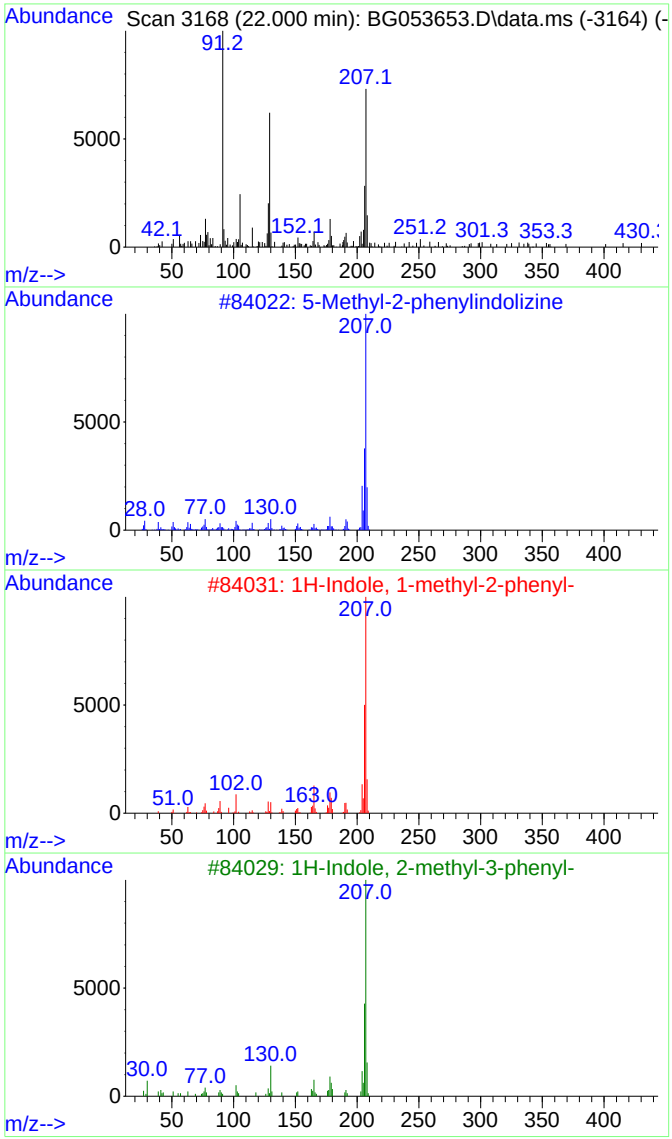
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

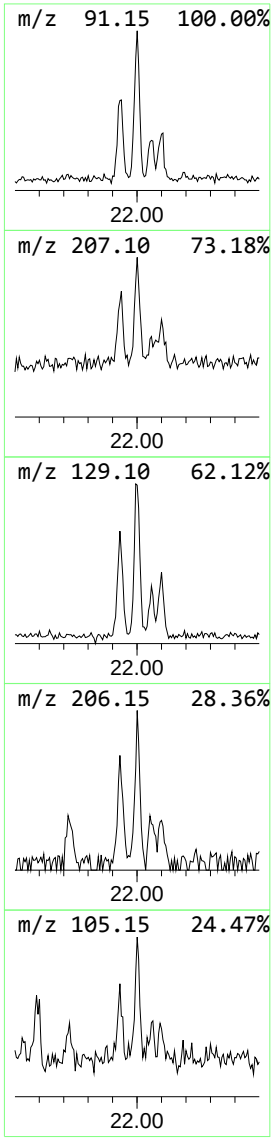
****

Peak Number 5 5-Methyl-2-phenylindolizine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.000	2.95 ng	84249	Chrysene-d12	21.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	53
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	52
3	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	49
4	1-benzylindole	207	C15H13N	1000334-31-3	45
5	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

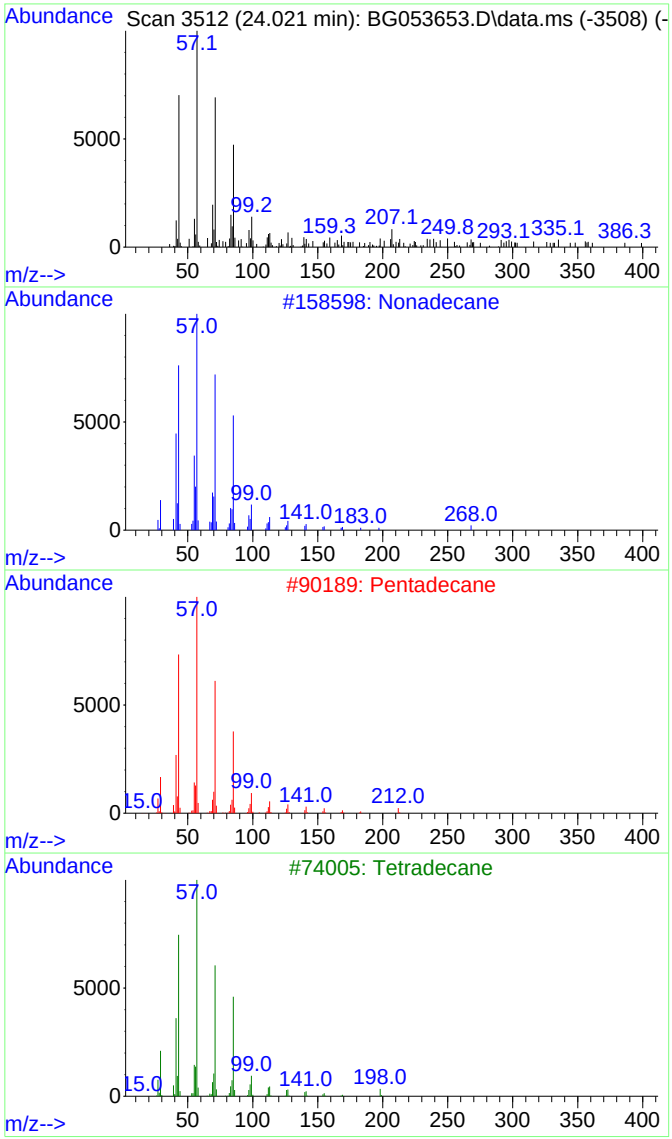
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

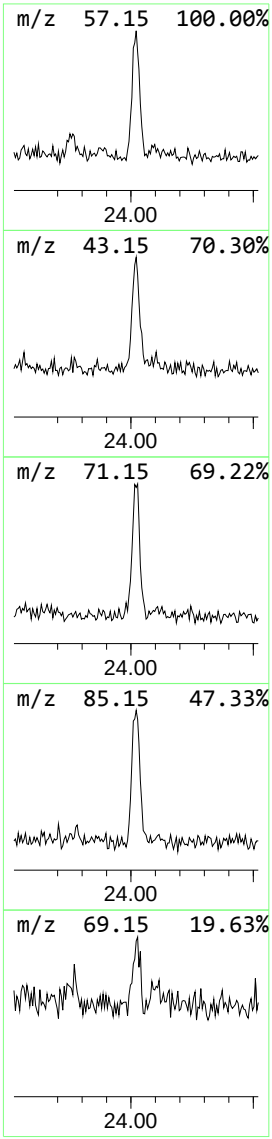
****

Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.021	3.87 ng	105392	Perylene-d12	24.990

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Pentadecane	212	C15H32	000629-62-9	83
3	Tetradecane	198	C14H30	000629-59-4	70
4	Eicosane	282	C20H42	000112-95-8	58
5	Succinic acid, 2,4,6-trichloroph...	380	C15H15Cl3O5	1000390-72-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

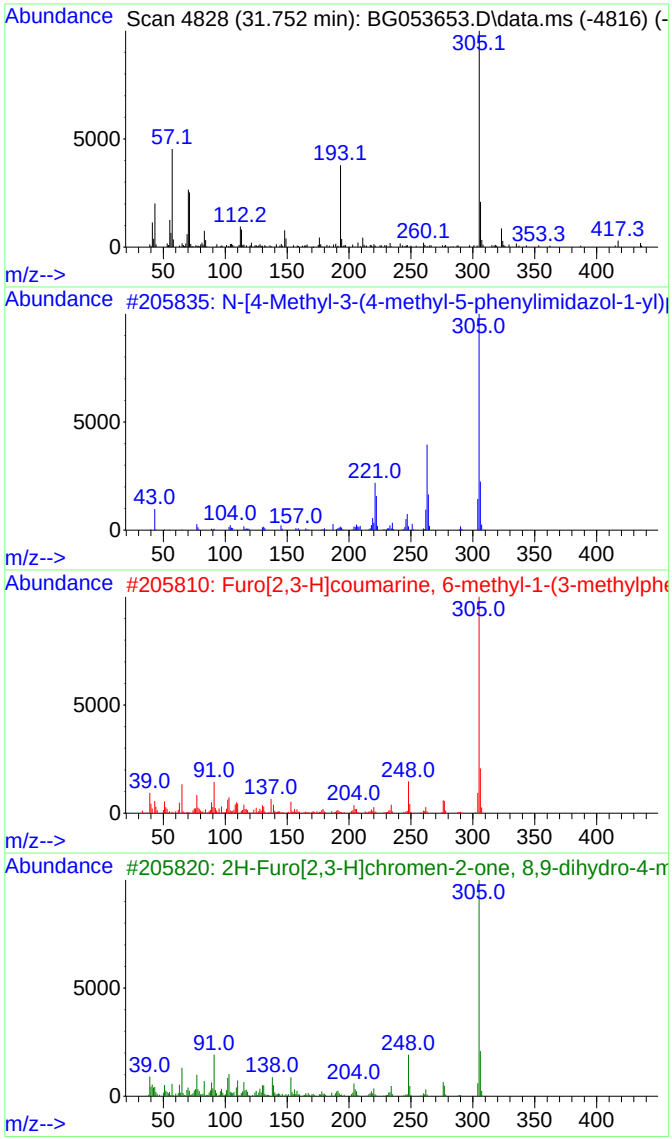
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

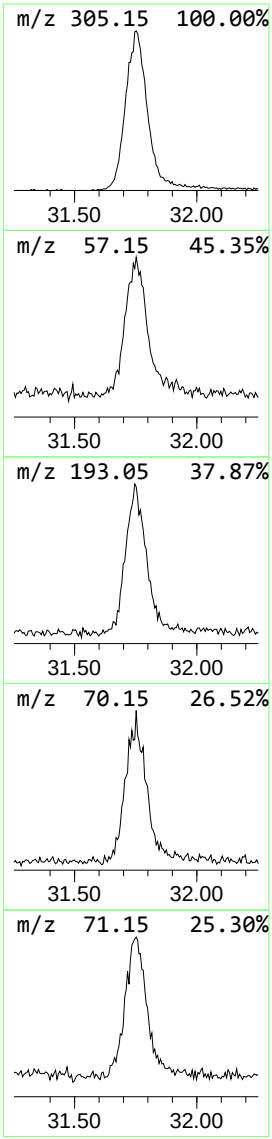
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown31.752 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.752	18.47 ng	503648	Perylene-d12	24.990

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[4-Methyl-3-(4-methyl-5-phenyl...	305	C19H19N3O	1000459-63-7	46
2	Furo[2,3-H]coumarine, 6-methyl-1...	305	C19H15NO3	1000270-15-3	46
3	2H-Furo[2,3-H]chromen-2-one, 8,9...	305	C19H15NO3	1000271-14-0	43
4	6-Methoxy-3-(p-methoxyphenyl)-9H...	305	C18H15N3O2	004460-54-2	43
5	Terephthalic acid, octyl 2-pheno...	398	C24H30O5	1000416-04-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052022\
Data File : BG053653.D
Acq On : 20 May 2022 21:02
Operator : CG/JU
Sample : N2865-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P019-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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-...	5.164	2.3	ng	28451	1	8.066	251074	20.0
unknown9.458	9.458	4.7	ng	58813	1	8.066	251074	20.0
n-Hexadecanoic ...	18.323	6.7	ng	177048	4	17.442	528403	20.0
unknown21.342	21.342	5.2	ng	146894	5	21.724	570690	20.0
5-Methyl-2-phen...	22.000	3.0	ng	84249	5	21.724	570690	20.0
Nonadecane	24.021	3.9	ng	105392	6	24.990	545314	20.0
unknown31.752	31.752	18.5	ng	503648	6	24.990	545314	20.0