LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.139	12	17	34	rVB	123940	242566	16.43%	2.530%
2	5.107	347	352	360	rBV	37276	63417	4.30%	0.662%
3	5.583	425	433	441	rBV	426515	705602	47.79%	7.361%
4	7.193	699	707	718	rBV	442000	792886	53.70%	8.272%
5	8.027	843	849	857	rVB2	107807	180871	12.25%	1.887%
6	9.196	1040	1048	1059	rBV	285757	515035	34.88%	5.373%
7	10.606	1283	1288	1300	rBV	39145	83189	5.63%	0.868%
8	10.847	1321	1329	1337	rBV	140750	254361	17.23%	2.654%
9	13.296	1739	1746	1754	rBV	674416	1061677	71.91%	11.076%
10	14.683	1974	1982	1989	rBV	222534	355536	24.08%	3.709%
11	16.175	2229	2236	2247	rBV	660122	1013709	68.66%	10.575%
12	17.432	2441	2450	2455	rBV	280787	439464	29.77%	4.585%
13	17.479	2455	2458	2465	rVB	82202	112042	7.59%	1.169%
14	17.567	2465	2473	2479	rBV	19595	33113	2.24%	0.345%
15	18.313	2594	2600	2604	rBV2	18071	25043	1.70%	0.261%
16	18.360	2604	2608	2615	rVB3	16714	26955	1.83%	0.281%
17	18.507	2627	2633	2637	rBV3	17405	30563	2.07%	0.319%
18	18.812	2678	2685	2689	rBV2	10484	18419	1.25%	0.192%
19	19.488	2795	2800	2805	rVB	152797	210703	14.27%	2.198%
20	19.823	2851	2857	2858	rBV3	28513	45549	3.09%	0.475%
21	19.846	2858	2861	2869	rVB	126825	187708	12.71%	1.958%
22	20.046	2888	2895	2900	rBV	1117800	1476427	100.00%	15.402%
23	20.169	2912	2916	2923	rVB5	12258	23708	1.61%	0.247%
24	20.316	2935	2941	2942	rBV7	10835	18735	1.27%	0.195%
25	20.334	2942	2944	2950	rVB3	20707	32013	2.17%	0.334%
26	20.439	2958	2962	2966	rBV4	13225	18011	1.22%	0.188%
27	20.498	2966	2972	2977	rVV6	12284	26440	1.79%	0.276%
28	21.103	3072	3075	3082	rBV6	8771	16846	1.14%	0.176%
29	21.285	3102	3106	3110	rBV6	10338	16336	1.11%	0.170%
30	21.350	3111	3117	3121	rBV6	34936	77504	5.25%	0.809%
31	21.444	3130	3133	3138	rVB5	13399	20253	1.37%	0.211%
32	21.714	3171	3179	3184	rVV2	280968	560864	37.99%	5.851%
33	21.761	3184	3187	3193	rVB2	56913	87238	5.91%	0.910%
34	21.908	3208	3212	3217	rBV6	10836	20532	1.39%	0.214%
35	22.454	3302	3305	3309	rVB4	13540	20920	1.42%	0.218%
36	23.952	3551	3560	3567	rBV2	37784	131404	8.90%	1.371%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.205	3599	3603	3611	rVB9	9702	21406	1.45%	0.223%
38	24.687	3678	3685	3691	rVB	24411	58318	3.95%	0.608%
39	24.834	3699	3710	3719	rBV2	38276	118886	8.05%	1.240%
40	24.986	3728	3736	3746	rVB3	144640	415994	28.18%	4.340%
41	29.891	4565	4571	4574	rBV8	12379	25472	1.73%	0.266%

Sum of corrected areas: 9585715

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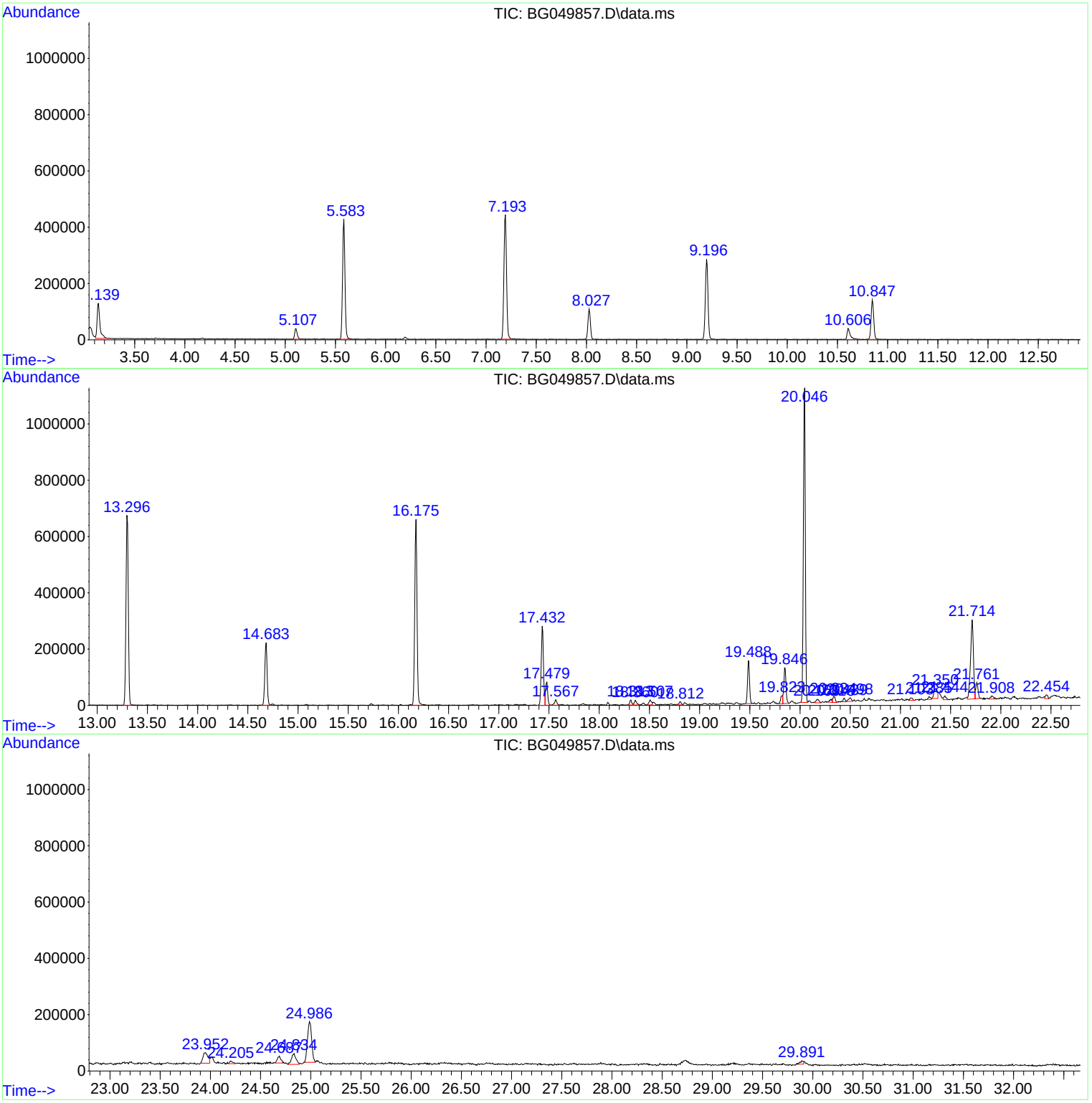
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
29S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
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Instrument : BNA_G
ClientSampleId : 29S

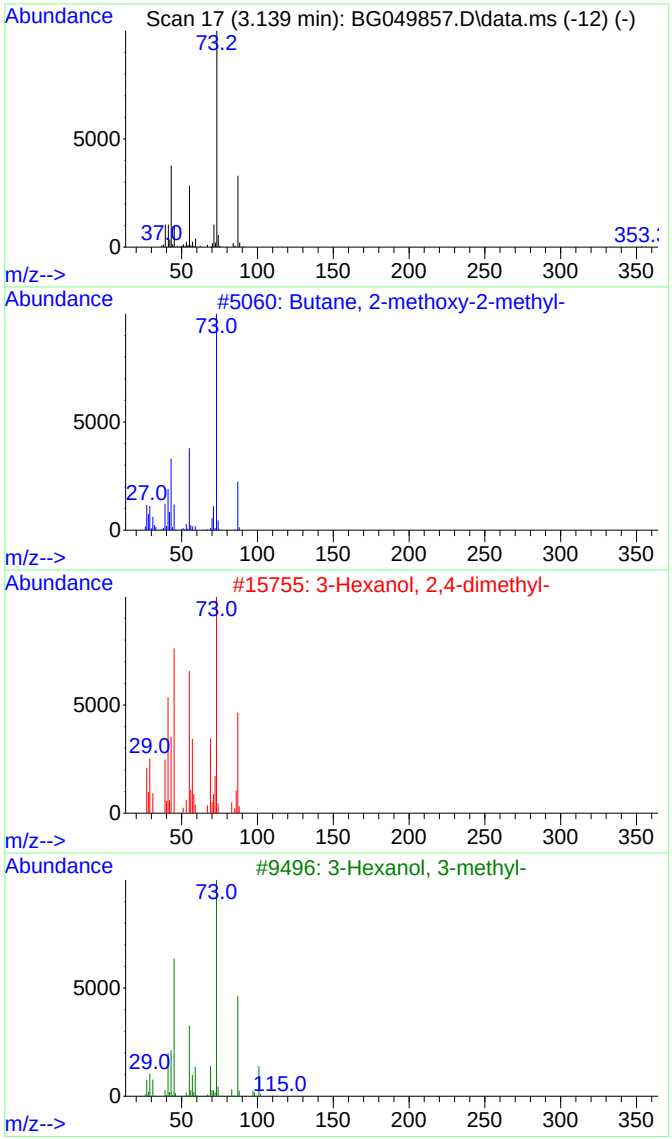
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

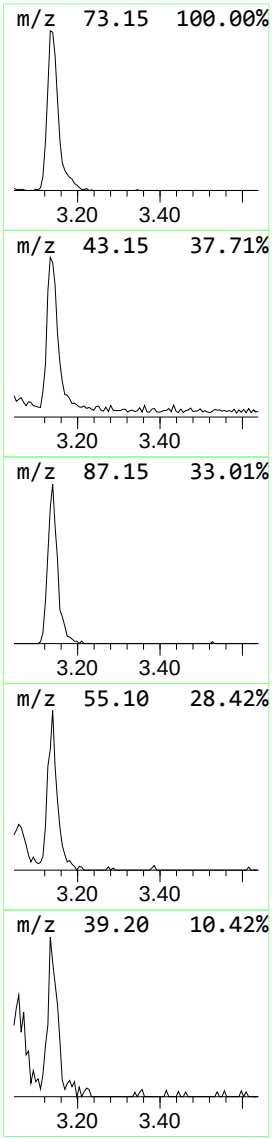
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.139	26.82 ng	242566	1,4-Dichlorobenzene-d4	8.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
3	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	38
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
5	Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

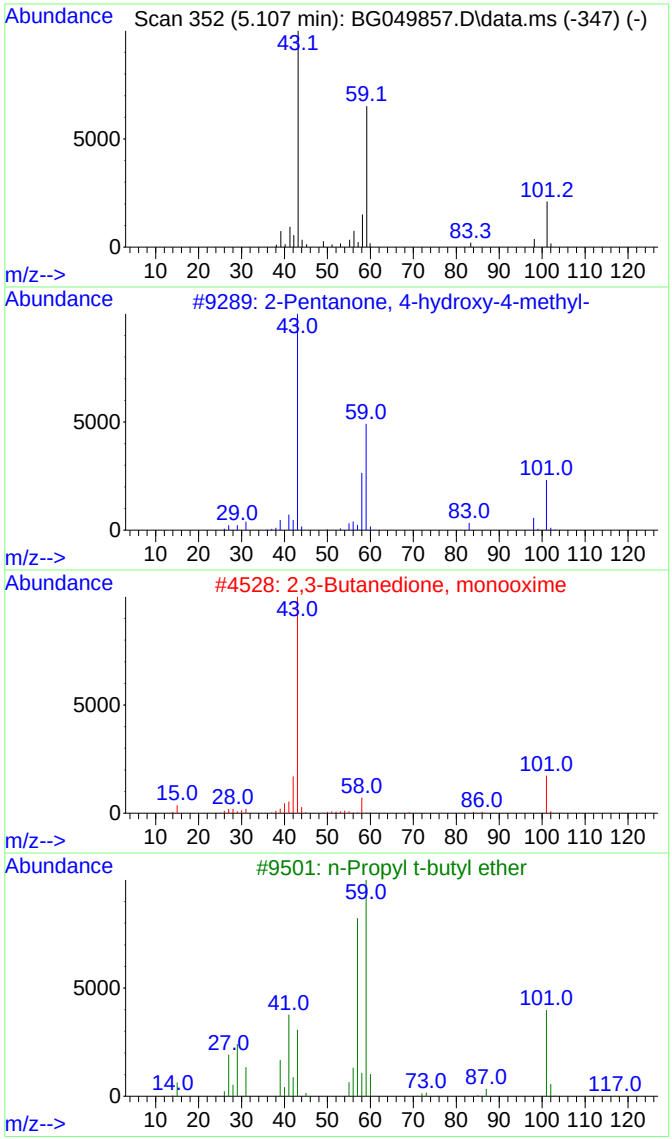
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

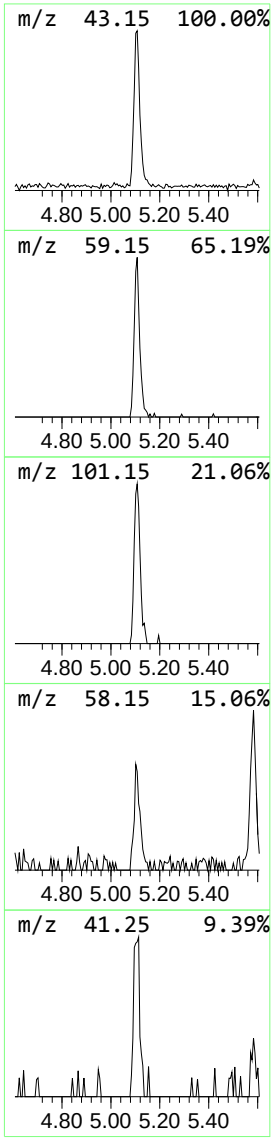
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.107	7.01 ng	63417	1,4-Dichlorobenzene-d4	8.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

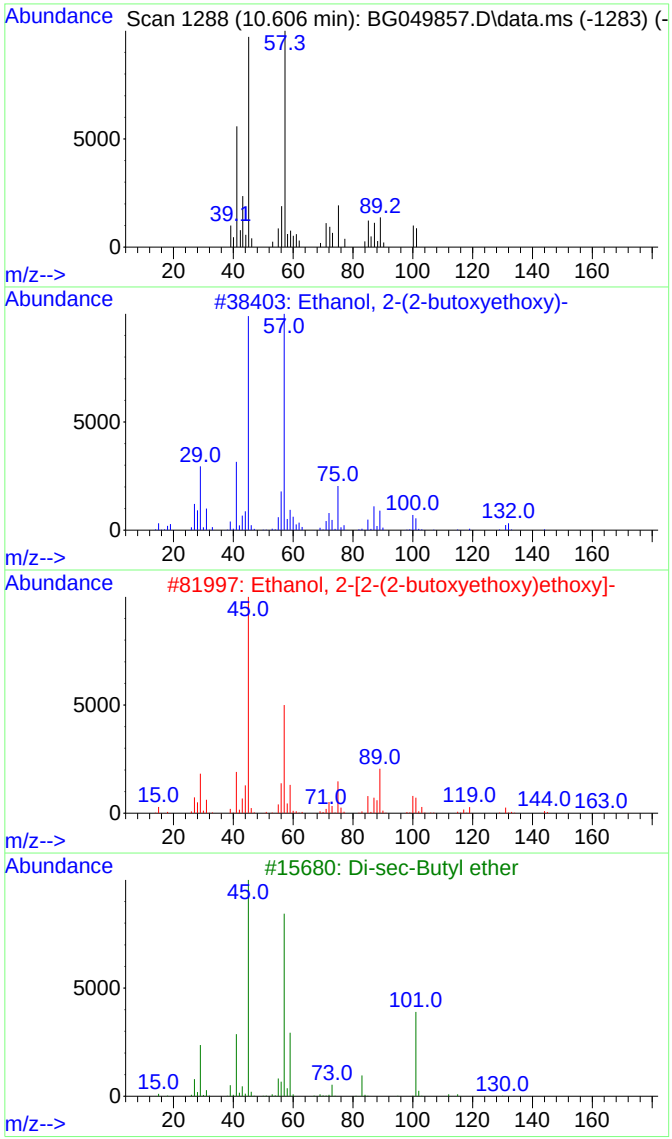
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

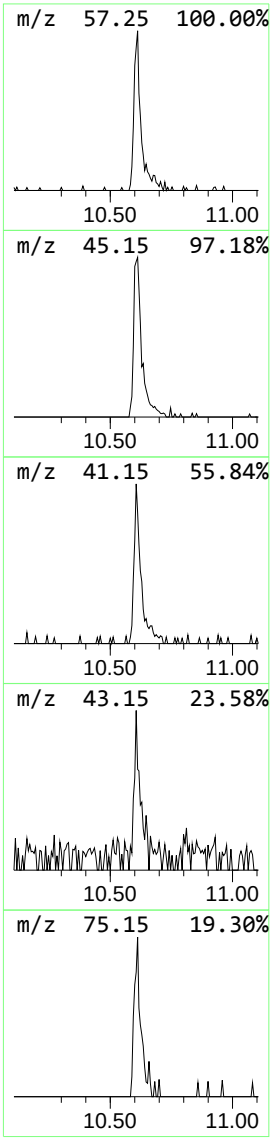
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.606	6.54 ng	83189	Naphthalene-d8	10.847

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	47
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049857.D
Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

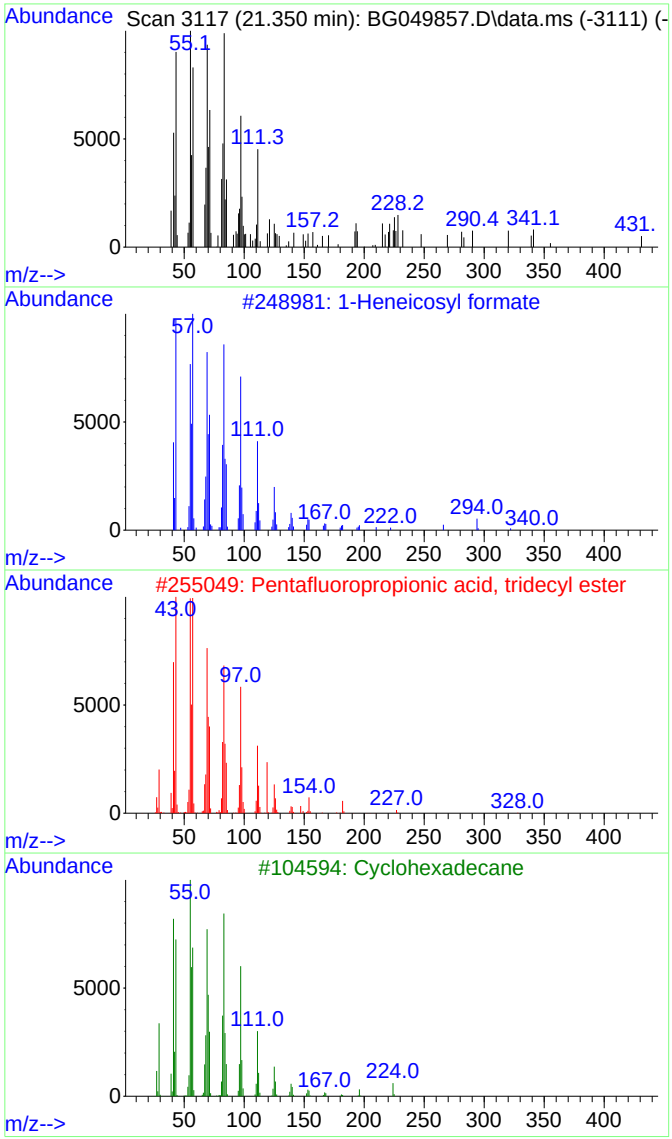
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

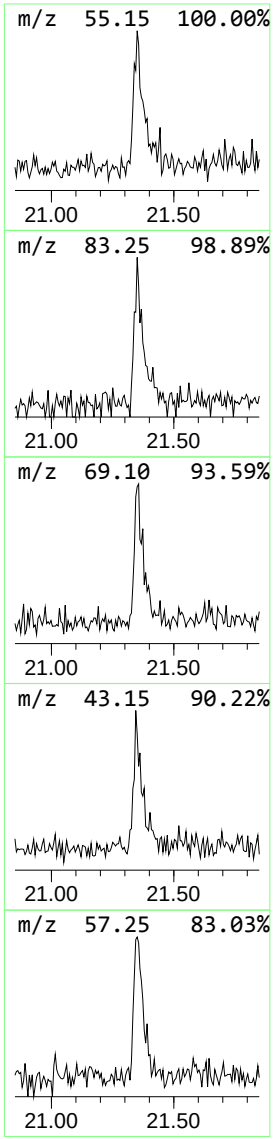
****

Peak Number 4 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.350	2.76 ng	77504	Chrysene-d12	21.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	86
2	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	86
3	Cyclohexadecane	224	C16H32	000295-65-8	81
4	Nonacos-1-ene	406	C29H58	018835-35-3	81
5	1-Methoxyoctacosane	424	C29H60O	237742-62-0	68





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Acq On : 16 Aug 2021 19:47
Operator : CG/JU
Sample : M3407-29
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 29S

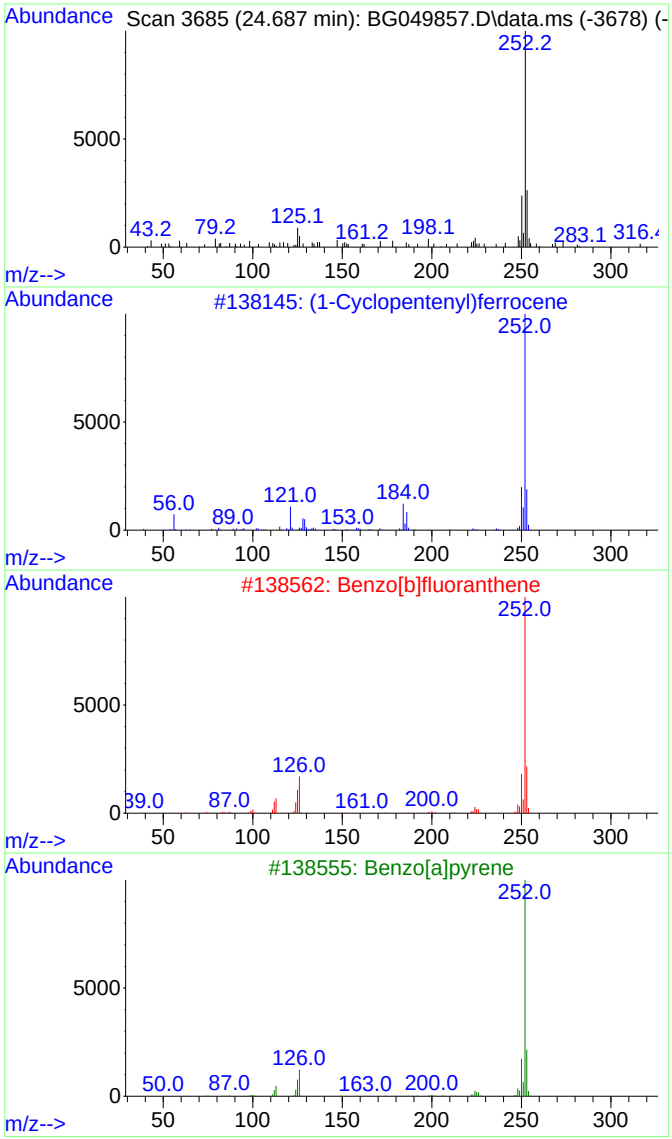
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

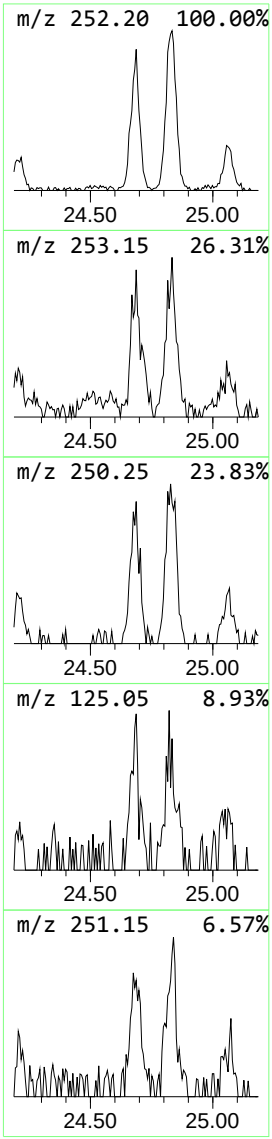
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (1-Cyclopentenyl)ferrocene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.687	2.80 ng	58318	Perylene-d12	24.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	74
3	Benzo[a]pyrene	252	C20H12	000050-32-8	74
4	Perylene	252	C20H12	000198-55-0	74
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
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Instrument : BNA_G
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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
Butane, 2-metho...	3.139	26.8	ng	242566	1	8.027	180871	20.0
2-Pentanone, 4-...	5.107	7.0	ng	63417	1	8.027	180871	20.0
Ethanol, 2-(2-b...	10.606	6.5	ng	83189	2	10.847	254361	20.0
1-Heneicosyl fo...	21.350	2.8	ng	77504	5	21.714	560864	20.0
(1-Cyclopenteny...	24.687	2.8	ng	58318	6	24.986	415994	20.0